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The principal objective of this study was to investigate process simulation and optimization of an existing offshore natural gas process which needed profitability improvements. Optimization was done using two alternative approaches: a global approach (response surface methodology) or a local approach (successive quadratic programming). The global approach was characterized by process performance at selected case study points throughout the feasible operating region and made use of *global information*, while the local approach was characterized by numerical iterative computation driven by *local information* in the neighborhood of a single point in the design space. A Box-Behnken design was used as a second-order response surface design for the estimation of correlation between process simulator design variables and an economic objective function, and the estimation model was then optimized. In the local approach, a process simulator (ASPEN PLUS) with optimization capabilities was used.

From the investigation, three major design variables were identified that had significant effects on the objective function of maximum product sales value. The three variables were: the compression ratio of the Production Compressor, the heat duty of the

Gas/Gas Exchanger, and the compression ratio of the Expander. The results indicated that profitability of the offshore natural gas process could be improved by greatly (about 60%) increasing the production of raw condensate, even though this meant slightly lower (about 4%) sales of natural gas as a main product. The improvement found, however, was only 7% when the design variables were limited by currently installed equipment.

The global approach was found to converge more consistently because once the global quadratic model was calculated, convergence to its unique optimum was simple. On the other hand the local approach had non-unique termination points due to the small effects of some design variables. The global approach provided better engineering insight since the effects of each design variable could be easily calculated from the quadratic model. However, the global approach was less efficient in terms of engineering manpower because of the time required to identify the quadratic model.

Simulation and Optimization of an Offshore Natural Gas Process

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Nopasit Chaiwanakupt, Author

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Nomenclature

Any italic letter indicates a scalar variable, while an italic letter with an underline indicates a set (vector) of variables.

List of Variables

A, B, C, D	=	Constants for analysis of Box-Behnken designs
C_c	=	Unit price of condensate (5.24 US$/ft^3)
C_g	=	Unit price of gas (3.60 US$/mmbtu)
D_i	=	Dependent variable
F	=	Volumetric flow of condensate at standard condition (ft^3/hr)
$f(\underline{x})$	=	Objective function
f_y	=	The RSM model of the economic objective
$\underline{g}(\underline{x})$	=	Inequality constraints
$\underline{h}(\underline{x})$	=	(1) Process equations
		(2) Equality constraints
$\underline{\underline{H}}$	=	Hessian matrix
k	=	Number of factors in experimental design
L	=	Lagrangian function
M	=	(1) Molar flow rate of sale gas (lbmol/hr)
		(2) Number of blocks for Box-Behnken designs
n	=	Number of experimental runs in each block

n_o	=	Number of center points
N	=	Number of all experimental runs
s	=	Number of manipulating variables in each run of Box-Behnken designs
v_i	=	Design variable
V	=	Regression variance
x_i	=	Normalized design variable
x_l	=	Lower bound on x
x_u	=	Upper bound on x
$\underline{X}$	=	Process variables
y	=	Standard response variable used in Box-Behnken design specification
$\underline{z}$	=	Freed variables

Greek Symbols

α	=	Step size
σ^2	=	Mean square of error
β	=	Polynomial coefficient
δ	=	Differences
∇	=	Gradient operator
λ	=	Lagrange multiplier

Subscripts

c	=	Condensate
g	=	Gas
i	=	Denotes variable i
j	=	Denotes variable j
k	=	Denotes values at kth iteration
l	=	Lower limit
o	=	Center point
u	=	(1) Upper limit
		(2) Denotes variable u
y	=	The RSM model of the economic objective, f_y

Simulation and Optimization of an Offshore Natural Gas Process

Chapter 1

Introduction

1.1 The Natural Gas Process

The process to be investigated was an offshore natural gas process in the Gulf of Thailand. The primary purpose of this process is to produce natural gas from offshore gas wells and send it to an onshore gas separation plant. In the past, efficiency of the process was not a major concern, because only one company produced natural gas in Thailand. Now, however, three companies are competing. To improve the efficiency, the process was studied using process simulation and then optimized by using only operating conditions plus one heat duty for an exchanger as the design variables. Units for physical variables were chosen to reflect common use in the natural gas industry.

1.2 Uses of Process Optimization

In recent years the chemical industry has been changed significantly due to increased costs of energy, limitations on natural resources, increasingly stringent environmental regulations and increased competition among manufacturers. Modification of plant design procedures and plant operating conditions have been implemented in order to reduce energy consumption, reduce other operating costs, maximize yield of valuable

products and meet improved safety constraints. In the near future emphasis will be on improving efficiency and increasing profitability of existing plants, rather than on plant expansion. One of the most powerful engineering tools that can be utilized in such activities is mathematical optimization. Process optimization can be used to improve yields from operating plants and to reduce maintenance costs, with less equipment wear and better staff utilization. Additionally, as computer technology continues to be developed and computers become even more powerful, even more problems can be solved by such optimization techniques.

Process optimization is valuable in different ways throughout three stages in the life of a project (Gallier and Kisala, 1987):

"***Process Development***: While evaluating process alternatives, it is important that any comparison be based on the optimum for each alternative. Frequently, simplified or shortcut models for the process can be used in early stages of the design, and rigorous models can then be used in later stages.

Plant Design: Once the process configuration is fixed, the results of the energy and material balance calculations are used to finalize the design of the process and its equipment. For this stage, detailed equipment sizes and costs, as well as operating costs are important in determining the optimum design.

Plant Operation: Optimization studies of existing plants can be important when there is variation in the feed to the plant or when the demand on production or product ratio change. Capital costs are then not important, and the optimization objective is based on production rate and operating costs."

This thesis describes an optimization project in the third stage, plant operation, with a simplified economic objective of maximizing the combined value of two products.

1.3 Process Simulation Software

In process optimization a model which accurately describes the process is required. Since the profitability and investment of a process are found from a model made up of numerous interacting parts, all the variables of the process must normally be considered simultaneously in order to find the most desirable combination. It is difficult to develop such an accurate model for large processes and such a model may require excessive computing time when used in optimization studies. Consequently, optimization of large or complex chemical processes often requires simplifying the system to reduce the mathematics to a form manageable by available algorithms or to reduce the time required to perform the computations. Such simplification, however, can alter the solution of the problem. Process simulators are ideally suited to the studies of chemical process optimization because they offer a convenient means to examine the entire process with an acceptable level of accuracy.

A process simulator may be defined as flow sheeting software that does physical property calculations and solves rate equations and steady-state material and energy balances. There are two basic alternatives for the mathematical formulation of problems encountered in flow sheeting software. The more general method is the ***equation-oriented*** method of solution. In this method, the entire set of equations and inequalities representing the process is employed simultaneously so that the process model equations

form the constraints for optimization. The more common alternative solution method is the ***modular*** method. In that method, the process is represented by a collection of modules, which are models of individual units in a flow sheet (such as a distillation column) that can be coded, analyzed, debugged, and interpreted individually. The equations representing each module are collected together and coded so that the module can be used in isolation from the rest of the flow sheet and hence is portable from one flow sheet to another.

Currently most commercial simulators are based on the sequential modular approach. The order in which the modules are calculated normally reflects the flow of material in the process and is thus rigidly defined by the topology of the flow sheet. Sequential modular process simulators are relatively easy to construct, analyze and run but also have some disadvantages. The rigidly defined calculation sequence makes them most useful only when doing performance or rating calculations. For optimization studies, they are usually considerably slower to converge because the simulator lacks flexibility in calculation order. On the other hand, the equation-oriented process simulators easily accommodate optimization calculations, but they are not able to handle problems with as many variables as those routinely handled by the sequential modular process simulators.

In current practice, optimization combined with modularly organized simulators seems to prevail because:

1. Individual modules are easy to construct and understand.
2. Addition and deletion of modules for a flow sheet is easily accomplished without changing the solution strategy.

3. Modules are easier to program and debug than sets of equations, and diagnostics for them are easier to analyze.
4. Many standard modules already exist.

1.4 Use of Process Simulation in Optimization

In the past, most process optimization was done with process simulation models on a "case study" basis. Several simulation cases were chosen by the engineer at different operating conditions, with the assumption that the "best" of these cases would be sufficiently "close" to the true optimum. As an alternative, the "best" can be calculated from an empirical model of the economic objective as a function of the design variables based on results of the case studies. Such an empirical model can be obtained by using a statistical tool called ***Response Surface Methodology (RSM)***. The response surface design chosen for this thesis is a Box-Behnken type which yields a second-order model. The optimum from this quadratic RSM model is then compared with results obtained from a process simulator which uses an internally coded ***Sequential Quadratic Programming (SQP)*** algorithm to find the optimum of the fundamental model based on physical properties, rate equations and mass and energy balances.

Both RSM and SQP approaches use second-degree polynomial models. For the RSM approach, the correlation between process simulator design variables and the economic objective function is based on *global* data from the appropriately chosen design cases. The SQP algorithm, on the other hand, sequentially minimizes a *local* quadratic model of the objective function, subject to constraints on the design variables. The SQP

algorithm attempts to converge to the global optimum by solving a series of local quadratic programs (QPs). The QP solution is used to generate a new search direction for the next iteration. A new step size is found along this direction to obtain an objective function improvement, subject to the design variable constraints. The computation is terminated when the objective function improvement is within a specified limit.

1.5 Scope of Investigations

The major goal of this work was to investigate the natural gas process through process simulation and optimization studies. Two process simulators were utilized: CHEMCAD III, developed by Chemstation, Inc., Houston, Texas and ASPEN PLUS, developed by Aspen Technology, Inc., Cambridge, Massachusetts.

The specific objectives of this work were to:

1. Simulate a natural gas processing plant at nominal design conditions using two commercial process simulators and compare predictions, speed and ease of use.
2. Compare the use of each process simulator to analyze and optimize the natural gas processing plant.
3. Determine the most important variables affecting the defined objective function in order to guide future experimental work with the actual process. If possible, develop simple operating principles which reflect profitability.

Chapter 2

Offshore Natural Gas Process

2.1 Process Description

The process to be optimized was an offshore natural gas process. Figure 2.1 is the process flow diagram with variables corresponding to the nominal design as calculated using the ASPEN PLUS simulator. In this process, a three-phase mixture from gas wells flows into the Inlet Separator, where gas, condensate, and water products are separated. The Inlet Separator is operated at 80 F and 315 psia. Condensate from the Inlet Separator goes to a condensate processing system to reduce its vapor pressure before being transported and stored in a floating storage unit. Water from the Inlet Separator goes to a water disposal system before it is pumped to the sea.

The gas product from the Inlet Separator flows to the Suction Scrubber, where any carry-over liquid in the gas flow is scrubbed in order to prevent liquid contamination downstream in the Production Compressor. This centrifugal compressor is used to raise the pressure of the gas flow to 1000 psia, after which it is cooled while passing through the Production Cooler.

Following the Production Cooler, the gas enters the Glycol Contactor (a dehydration unit), where the water content in the gas flow is reduced. The maximum allowable water content in product gas for a subsea pipeline is 10 ppm. Glycol used in

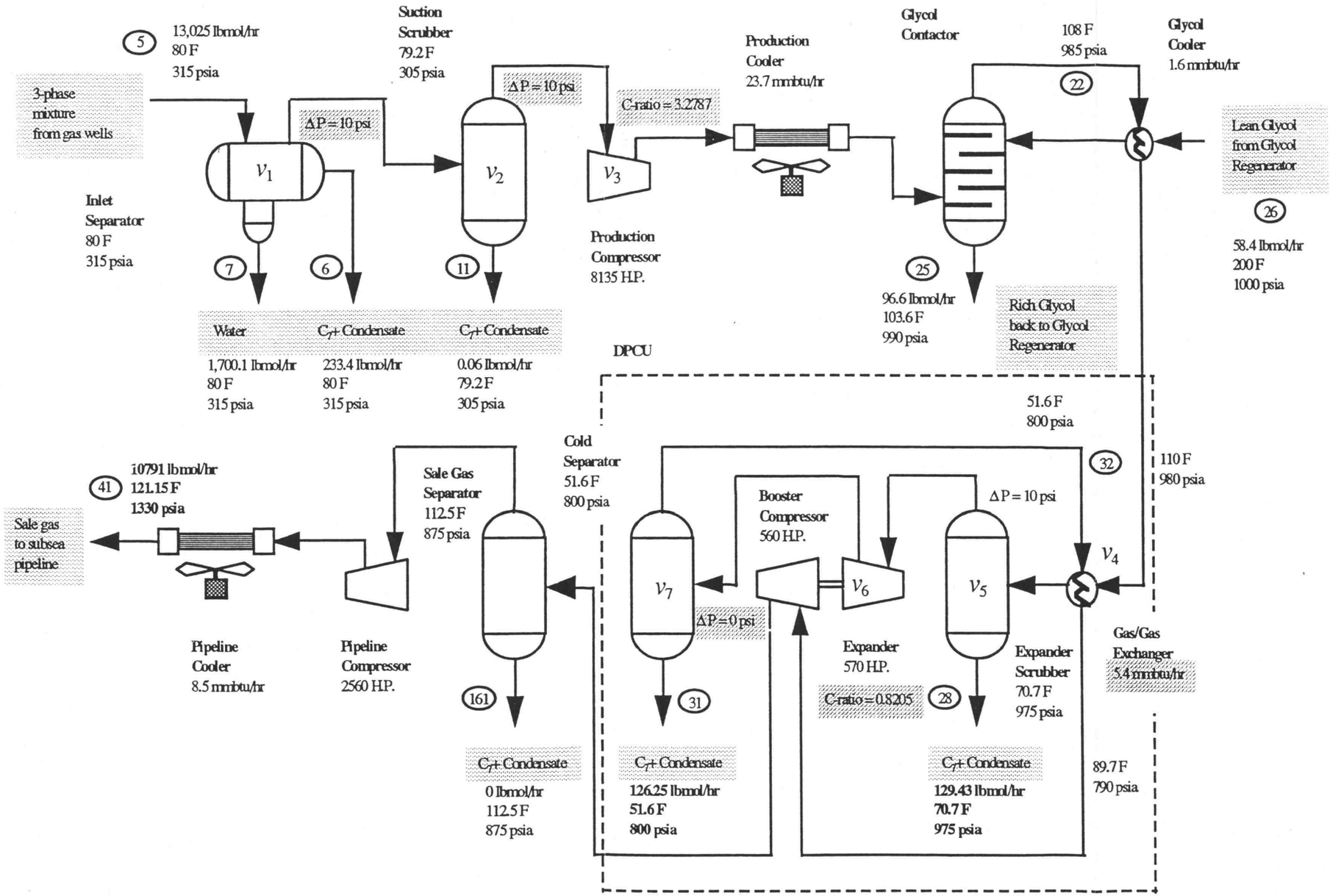

Figure 2.1 Flow diagram of the natural gas process - nominal design (ASPEN PLUS)

this unit is Tri-Ethylene-Glycol (TEG). Lean glycol from a Glycol Regenerator is cooled through a heat exchanger prior to entering the Glycol Contactor. The rich glycol product from the Glycol Contactor is returned to the glycol regeneration unit.

The dehydrated gas is heated in the Gas/Gas Exchanger and enters the Dew Point Control Unit (DPCU). The DPCU consists of five units: one heat exchanger, one expander, one compressor, and two separators. Its objective is to lower the dew point temperature of the gas flow to 50 F at atmospheric pressure, which is the maximum allowed for the subsea pipeline. At first the gas flows through the Gas/Gas Exchanger and is cooled by the gas flow from the Cold Separator. From the Gas/Gas Exchanger, the gas flow enters the Expander Scrubber to remove any condensed liquid which would damage the Expander due to liquid contamination. The gas flow then goes through the Expander. Pressure and temperature at the outlet from the expander decrease to 800 psia and 50 F, respectively, so that the discharge flow contains some condensate, which is removed in the Cold Separator. As a result of condensate removal, the dew point of the gas flow is lowered to its required value. After the Cold Separator, the gas flow is heated up as it flows through the Gas/Gas Exchanger, to make sure that there is no liquid contamination in the gas flow before entering the Booster Compressor where the pressure is raised to 875 psia. After leaving the Booster compressor, the compressed gas then enters the Sale Gas Separator.

In the Sale Gas Separator, any remaining liquid contaminants are removed and the gas flow is then pumped to the Pipeline Compressor to increase its pressure above the

pipeline level. From the Pipeline Compressor, the gas enters the Pipeline Cooler after which it is sent to the subsea pipeline.

2.2 Economic Objective

There are many criteria used in economic analysis in the chemical process industries. The best known criteria are the payback period (PBP), return on investment (ROI), internal rate of return (IRR), and net present value (NPV). In order to perform any detailed economic evaluation, the following parameters have to be specified: initial investment, future cash flows, salvage value, economic life, depreciation, depletion, tax credit, taxes, inflation, and debt/equity ratio.

For this study, the chosen plant was an existing plant for which the cost of capital investment was already recovered. Moreover, most of the manipulated variables were operating conditions, which would not require any investment. The manipulated variable that implied a plant modification, the heat duty of the Gas/Gas Exchanger, would require a relatively small amount of investment. Since operating costs were considered to be nearly constant, a simple but useful criterion for measuring profitability was total sales.

Total sales of the natural gas process consist of sales of gas and condensate. The unit price of gas and condensate were assigned to be 3.60 US$/mmbtu(gross) and 5.24 US$/ ft^3 (std), respectively. Note that 1 mmbtu = $1x10^6$ btu. In this study, total sales were considered on a daily basis (24 hours of continuous operation).

The objective function, f, was based on stream variables calculated by the process simulator. In this study the objective function was chosen as the total dollar sales of sale gas and raw condensate per day.

$$\text{Sales} = f = \left[M_{g,41} Q_g C_g + \left(F_{c,6} + F_{c,11} + F_{c,28} + F_{c,31} + F_{c,161}\right) C_c\right] \times 24 \qquad (2.1)$$

where:

$M_{g,41}$ = Molar flow rate of sale gas, stream 41 (lbmol/hr)

$F_{c,i}$ = Standard volumetric flow rate of stream # i (ft^3/hr)

i = 6, condensate from Inlet Separator

i = 11, condensate from Suction Scrubber

i = 28, condensate from Expander Scrubber

i = 31, condensate from Cold Separator

i = 161, condensate from Sale Gas Separator

Q_g = Gross heating value of sale gas (mmbtu/lbmol)

C_g = Unit price of sale gas (3.60 US$/mmbtu)

C_c = Unit price of condensate (5.24 US$/$ft^3$)

All variables in the objective function are functions of the design variables.

2.3 Process Optimization Statement

To maximize total sale of natural gas and raw condensate per day, seven design variables (v_1-v_7) were chosen and the optimization problem was thus stated as:

$$\text{Max} \quad Sales = f(v_1, v_2, \ldots, v_7) \tag{2.2}$$

Subject to:

$$v_1 \leq 20$$

$$v_2 \leq 20$$

$$2.951 \leq v_3 \leq 3.607$$

$$3.625 \leq v_4 \leq 7.250$$

$$v_5 \leq 20$$

$$0.656 \leq v_6 \leq 0.985$$

$$v_7 \leq 20$$

$$D_1 \leq 65$$

$$D_2 \leq 10$$

$$v_1, v_2, \ldots, v_7, D_1, D_2 \geq 0$$

where:

v_1 = Pressure drop from Inlet Header to Inlet Separator (psi)

v_2 = Pressure drop from Inlet Separator to Suction Scrubber (psi)

v_3 = Compression ratio of Production Compressor

	=	Outlet pressure/inlet pressure
v_4	=	Heat duty of Gas/Gas Exchanger (mmbtu/hr)
v_5	=	Pressure drop from Gas/Gas Exchanger to Expander scrubber (psi)
v_6	=	Compression ratio of Expander
v_7	=	Pressure drop from Expander to Cold Separator (psi)
D_1	=	Standard dew point temperature of sale gas (F)
D_2	=	Water content in sale gas (ppm)

Constraints and bounds on the design variables, *v*'s, and the product specifications (implicit dependent variables), *D*'s, are maximum and minimum allowable operating conditions for the process.

Pressure drops in the Inlet Separator, the Suction Scrubber, the Expander Scrubber and the Cold Separator were used as design variables instead of operating pressures because they were independent to inlet pressure of each vessel, while the operating pressure could not be higher than the inlet pressure. The pressure drop could be manipulated by adjusting a pressure control valve at each vessel, with a minimum value dependent on the units physical design. Since the minimum and nominal design pressure drops were assumed to be 0 and 10 psi, respectively, the maximum pressure drop was set at 20 psi in order to have the pressure drops as equally-spaced three-level design variables.

The maximum compression ratios of the Production Compressor and the Expander were 3.607 and 0.985, respectively. These numbers reflected the maximum design for pressure outlet piping from the Production Compressor and the Expander, respectively,

when maximum inlet pressures were used. As the maximum and nominal design values were known, the minimum compression ratios were chosen so that the nominal values were the midpoints of the feasible ranges.

The Gas/Gas exchanger consisted of four shell-and-tubes units in parallel. Only three of these units were operated at nominal design condition. Since the heat duty of each unit was 1.8125 mmbtu/hr, the nominal heat duty is 5.4375 mmbtu/hr and the maximum heating value was assumed to be 7.25 mmbtu/hr. To make the nominal value the midpoint, the minimum value was assumed to be 3.625 mmbtu/hr.

Chapter 3

Traditional Optimization from Case Studies/Simulations

3.1 **Response Surface Methodology**

Response surface methodology (RSM) is a collection of tools developed in the 1950s for the purpose of determining optimum operating conditions. In a review of RSM techniques, Myers et al.(1989) observed that RSM was applicable to many fields of research, such as engineering sciences, food sciences, and biological and clinical sciences. .

The experimental design strategy of RSM is based on the assumption that a response f_y, e.g. the RSM model of the economic objective, is a function of a set of design variables $x_1, x_2,..., x_k$ and that the function can be adequately approximated in a region by a polynomial model in the x' s. The simplest models considered are the first-order model

$$f_y = \beta_0 + \beta_1 x_1 + ... + \beta_k x_k \tag{3.1}$$

and the second-order model

$$f_y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{\substack{i=1 \\ i<j}}^{k} \sum_{j=1}^{k} \beta_{ij} x_i x_j \tag{3.2}$$

In general any continuous function having derivatives of all orders in the interval being considered can be approximated by a Taylor series, no matter how complex the function may be. If the function is very complex, many terms may be needed in the Taylor series. When a known function is expanded in a Taylor series about a point, the error is zero at that point.

Box and Behnken (1960) stated that a second-order Taylor series is an adequate approximation in the operable region of most processes. However, the error is not likely to be small at points some distance from the point of expansion if only second-order terms are retained. In RSM, the coefficients in the polynomial model are not those of the local Taylor series, but are adjusted by the use of least squares to give a small prediction error throughout the region of interest. The region of interest is here assumed to be the region in which data (response values of f_y) have been obtained.

The polynomial approximation for a particular process is obtained by running an experiment in the independent (design) variables, x' s, and observing the dependent variables (responses), f_y's. These observations on the f_y's are then used to obtain estimates of the coefficients (β' s) shown in the general model. The β' s obtained are those that will result in an equation that will fit the data observed in the least squares sense.

The resulting polynomial approximation usually can be used for interpolation in the region in which the data were collected with only small errors. However, extrapolation may be much less accurate. Poorer accuracy is expected with extrapolation when the prediction point is far removed from the data used to generate the model. Consequently, the data should cover the entire region in which prediction will be made.

Since second-order effects are to be estimated, the experimental design must have at least three levels for each independent variable. It would be feasible to use the full three-level factorials which would provide orthogonal estimates of the linear, quadratic and interaction effects. However, a disadvantage of the full three-level factorials is the large number of experimental trials or runs required. The number of required runs (n) involving k factors is shown in Table 3.1.

Table 3.1 Number of runs required, n,in full three-level factorial design involving k factors

No.of Independent Variables (Factors), k	No. of Coefficients in Full Quadratic	No. of Runs in Full 3-Level Factorial (n)
2	6	9
3	10	27
4	15	81
5	21	243
6	28	729

The middle column of Table 3.1 shows the number of coefficients in the full quadratic polynomial model that must be determined from the data. This is also the absolute minimum number of experimental runs required. In reality, the number of data points generated is chosen to be greater than the minimum in order to provide degrees of

freedom from which an estimate of the error variance can be obtained. For every experimental run beyond the minimum number, an additional degree of freedom for error is obtained, and additional capacity is provided for the fitted equation to smooth out the random experimental errors when fitting a response surface. Thus, a good experimental design must provide reasonable, but not excessive, number of degrees of freedom for error.

In RSM, the concept of the prediction-variance profile is a relevant criterion in selecting a design (Box, 1954). It is desirable that the precision (i.e. variance) of the prediction be independent of the direction of any point from the center. Designs having this property are called "rotatable" designs. It is also desirable that the prediction variance be relatively constant at varying distances from the center of the design out to the boundary of the experimental region. In combination, these two properties produce a relatively constant prediction variance throughout the experimental region.

Another desirable feature of an experimental design when many runs are required is the feasibility of performing the experiments in separate "blocks" of runs ("block" is a set of experimental runs in which only a few of the design variables are changed.). This is especially useful when experiment modifications are required to change a design variable's value.

Although three levels is the minimum number for each factor, it is possible to develop designs using more than three-levels (Lucas, 1976). For example, central composite designs employ five levels of each factor. Of course it is often experimentally convenient to use only the minimum number of levels necessary. The Box-Behnken

designs (Box and Behnken, 1960) have this property and have been used successfully since they were published. These designs are some of the best second-order designs, in term of performance, and give good results in a wide range of practical problems (Lucas, 1976). The practical advantage of second-order Box-Behnken designs is that they require only three levels for each factor. All of the design points are either at the center of the design variable space or on a "spherical" surface (equidistant from the center). In Figure 3.1, the geometry of the Box-Behnken design for three factors is shown. The designs are either rotatable or nearly rotatable. In this work, the "Box-Behnken" design was employed for building an empirical model of the objective function for the operation of a natural gas processing plant. Although, the computer process simulator does not produce significant random errors, the "excess" objective function evaluations were considered useful in approximating the nonlinear behavior with the simple quadratic model.

3.2 Box-Behnken Experimental Designs

3.2.1 The Design

Each Box-Behnken design employs a subset of the points in the corresponding full three-level factorial. For example, the three-factor design shown in Figure 3.1 uses 13 of 27 points from the full factorial with two extra replicates at the center point, for a total of 15 points (see Table 3.2). This is five more than the minimum number of experimental runs required, therefore it provides five degrees of freedom for experimental or modeling error.

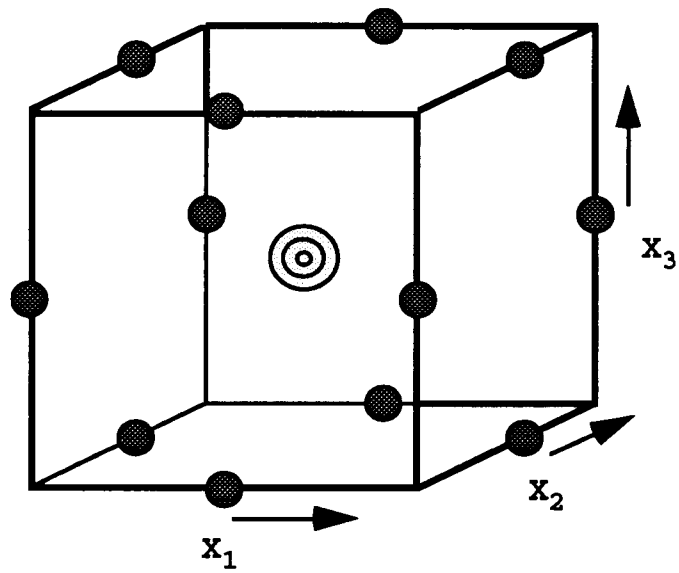

Figure 3.1 Geometry of Box-Behnken design for three variables

It is instructive to consider the geometric character of the array of points called for by the Box-Behnken designs. All points, except the center points, are at the midpoints of the edges (or faces) of a hypercube whose dimension is the number of factors, *k*. All of these points definitely lie on a single sphere and are, accordingly, equally distant from the center. This is a geometry property associated with rotatability, where rotatability is one of the desirable properties of a design. The replicated center points have two extra functions. The first function is to provide a measure of the inherent experimental error, when measurements are involved. The second function is to give sufficient number of experimental runs in order to offer relatively constant prediction variance as a function of distance from the center, within the design region. The prediction variance increases quite

Table 3.2 Three-factor Box-Behnken design

x_1	x_2	x_3	
+1	+1	0	
+1	−1	0	
−1	+1	0	
−1	−1	0	
+1	0	+1	
+1	0	−1	
−1	0	+1	
−1	0	−1	
0	+1	+1	
0	+1	−1	
0	−1	+1	
0	−1	−1	
0	0	0	Center points
0	0	0	
0	0	0	

rapidly with additional extrapolation distance from the center at the edge of region and beyond. For further theoretical details, it is recommended to see Box-Behnken, 1960.

Orthogonal blocking is another desirable feature of a design. If a large number of experimental runs is involved, it is desirable to run them in separate blocks of points, with the property of being able to subtract out the effect of a shift of response between blocks. This shifting effect causes a bias in the estimates of any of the polynomial coefficients. Design of this type provides "orthogonal blocking". Box-Behnken designs provide for orthogonal blocking into at least two blocks for four to ten factors.

Table 3.3 describes Design #1 to Design #4 which are useful for $k = 3$, 4, 5, and 7 (used for the natural gas process) factors, respectively. The design matrices shown in Table 3.3 are given in short-handed format. The two ± 1 in every row of the design #1, #2, and #3 are replaced by two columns of the two-level 2^2 design (for example, compare the three-factor Box-Behnken design given in Tables 3.2 and 3.3). Similarly, the three ± 1 in every row of the design #4 are replaced by three columns of the two-level 3^2 design.

3.2.2 Analysis for the Designs

The second-order empirical model was fitted by using the method of least squares. The model to be fitted was

$$f_y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{\substack{i=1 \\ i<j}}^{k} \sum_{j=1}^{k} \beta_{ij} x_i x_j$$

Formulae and constants for the designs of Table 3.3 are given in Tables 3.4 and 3.5, as derived by Box and Behnken, where $y = f_y$ for this thesis. The notation in the table is thus in terms of a standard response y, whereas the specific response in these studies was the economic objective, f.

Table 3.3 Some useful three-level designs

Design #	No. of Factors, k	Design Matrix	No. of Points	Blocking and Association Schemes
1	3	$\begin{bmatrix} \pm1 & \pm1 & 0 \\ \pm1 & 0 & \pm1 \\ 0 & \pm1 & \pm1 \\ 0 & 0 & 0 \end{bmatrix}$	12 3 $N=15$	No orthogonal blocking
2	4	$\begin{bmatrix} \pm1 & \pm1 & 0 & 0 \\ 0 & 0 & \pm1 & \pm1 \\ 0 & 0 & 0 & 0 \\ \pm1 & 0 & 0 & \pm1 \\ 0 & \pm1 & \pm1 & 0 \\ 0 & 0 & 0 & 0 \\ \pm1 & 0 & \pm1 & 0 \\ 0 & \pm1 & 0 & \pm1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	8 1 8 1 8 1 $N=27$	3 blocks of 9
3	5	$\begin{bmatrix} \pm1 & \pm1 & 0 & 0 & 0 \\ 0 & 0 & \pm1 & \pm1 & 0 \\ 0 & \pm1 & 0 & 0 & \pm1 \\ \pm1 & 0 & \pm1 & 0 & 0 \\ 0 & 0 & 0 & \pm1 & \pm1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \pm1 & \pm1 & 0 & 0 \\ \pm1 & 0 & 0 & \pm1 & 0 \\ 0 & 0 & \pm1 & 0 & \pm1 \\ \pm1 & 0 & 0 & 0 & \pm1 \\ 0 & \pm1 & 0 & \pm1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	20 3 20 3 $N=46$	2 blocks of 23

Table 3.3 Some useful three-level designs (continued)

Design #	No. of Factors, k	Design Matrix	No. of Points	Blocking and Association Schemes
4	7	$\begin{bmatrix} 0 & 0 & 0 & \pm1 & \pm1 & \pm1 & 0 \\ \pm1 & 0 & 0 & 0 & 0 & \pm1 & \pm1 \\ 0 & \pm1 & 0 & 0 & \pm1 & 0 & \pm1 \\ \pm1 & \pm1 & 0 & \pm1 & 0 & 0 & 0 \\ 0 & 0 & \pm1 & \pm1 & 0 & 0 & \pm1 \\ \pm1 & 0 & \pm1 & 0 & \pm1 & 0 & 0 \\ 0 & \pm1 & \pm1 & 0 & 0 & \pm1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	56 6 $N = 62$	2 blocks of 31

Table 3.4 Constants for the designs of Table 3.3

Design #	A	B	C	D	s	n_0
1	1/8	3/16	-1/16	1/4	2	3
2	1/12	5/48	-1/48	1/4	2	3
3	1/16	7/96	-1/96	1/4	2	6
4	1/24	1/18	-1/144	1/8	3	6

Note : n_0 = number of center points in the design

Table 3.5 Estimates of regression coefficients

Coefficients
$\beta_0 = \bar{y}_0 = \frac{\sum_i^N y_i}{N}$ $\beta_i = A\{iy\}$ $\beta_{ii} = B\{iiy\} + C\sum_j^{n_1}\{jjy\} - (\bar{y}_0 / s)$ $\beta_{ij} = D\{ijy\}$

$$\{iy\} = \sum_{u=1}^{N} x_{iu} y_u \tag{3.3}$$

$$\{iiy\} = \sum_{u=1}^{N} x_{iu}^2 y_u \tag{3.4}$$

$$\{ijy\} = \sum_{u=1}^{N} x_{iu} x_{ju} y_u \tag{3.5}$$

$$\{0y\} = \sum_{u=1}^{N} y_u \tag{3.6}$$

where

N = Number of experimental runs

For the designs which have multiple blocks, block effects must be eliminated. Since the blocking is orthogonal, the elimination of blocks will only affect the residual sum of squares. The sum of squares associated with blocks is

$$\frac{\sum_{m=1}^{M}\left(\overline{y}_m\right)^2}{n} - \frac{\{0y\}^2}{N} \tag{3.7}$$

where

n = Number of experimental runs in each block

M = Number of blocks

The variances and covariances of the various estimates can be obtained from the formulae in Appendix C.

3.3 Application to the Natural Gas Problem

The concept of this approach is to obtain a second-degree polynomial approximation that represents the objective function as a function of design variables by using response surface techniques on results from the process simulation software. The resultant quadratic optimization problem can then be easily solved. The following steps are required:

STEP 1: Plan a set of simulation experiments, utilizing the Box-Behnken design as the basis for a second-order response surface design.

STEP 2: Conduct the simulations and obtain values for the response variable (economic objective, f value).

STEP 3: Estimate the second-order polynomial used as the objective model (f_y) via a least-squares regression.

STEP 4: Determine optimal values for the design variables to maximize f_y.

As described in the process optimization statement, there are seven design variables for this problem. In order to avoid numerical scaling problems, normalized design variables were introduced at this step. Each of the seven design variables were normalized to range from -1 to +1 using the equation

$$x_i = \frac{v_i - \left(v_{i,\max} + v_{i,\min}\right)/2}{\left(v_{i,\max} - v_{i,\min}\right)/2} \tag{3.8}$$

As the Box-Behnken design is an equally-spaced three-factor design, the three levels chosen were -1, 0, and +1. Table 3.6 shows prenormalization values of design variables at these three levels. The nominal process design was represented by all $x_i = 0$.

Table 3.6 Numerical Values of Decision Variables at Three Levels

Coded Variable	Design Variable	Unit	Numerical Value at Each of 3 Levels		
			-1	0	+1
x_1	v_1	psi	0	10	20
x_2	v_2	psi	0	10	20
x_3	v_3	dimensionless	2.9508	3.2787	3.6066
x_4	v_4	mmbtu/hr	3.625	5.438	7.250
x_5	v_5	psi	0	10	20
x_6	v_6	dimensionless	0.6564	0.8205	0.9846
x_7	v_7	psi	0	10	20

STEP 1

Since this is a three-level seven-factor problem, the Box-Behnken design #4 (k = 7) in Table 3.3 was used.

STEP 2

The natural gas process was simulated using CHEMCAD III. The process simulator was treated as a "black box", i.e. only the objective function values were used to fit the quadratic model as a function of decision variables. The order of the experimental runs was randomized before running. Results of these simulations are discussed in Chapter 5.

STEP 3

From the experimental results, the second-order polynomial model was estimated using the formulae given in Tables 3.4 and 3.5. The values of the βs and their standard errors, and the analysis of variance for this experiment are reported in Chapter 5.

STEP 4

In this step, the maximum of the second-order polynomial model from the previous step was computed. The optimization statement for this approach can be written as:

$$\text{Max} \quad f_y = \beta_0 + \sum_{i=1}^{7} \beta_i x_i + \sum_{i=1}^{7} \beta_{ii} x_i^2 + \sum_{\substack{i=1 \\ i<j}}^{7} \sum_{j=1}^{7} \beta_{ij} x_i x_j \qquad (3.9)$$

subject to $-1 \leq x_i \leq 1$; i = 1,2,...,7

This optimization problem could have been solved by using quadratic programming (QP). Nevertheless, it was convenient to use a standard mathematical software, MATLAB, developed by Mathwork, Inc. (Natick, Massachusetts). One of the optimization algorithms available in the MATLAB optimization toolbox is SQP. Since this is a quadratic problem with linear constraints, this SQP method solves it in one step, as shown in Chapter 5. The MATLAB computer program written to solve this optimization problem is listed in Appendix A.

Chapter 4

Improved Process Optimization Using Process Simulators

Computer simulation has proved to be an extremely successful engineering tool for the design and operation of chemical processes for two decades, because the mathematical optimization of process simulation can bring about significant economic benefits (Squires and Reklaitis, 1980). As computer technology and modern optimization algorithms have been developed, optimization using process simulation has become even more effective.

4.1 Sequential Modular Process Simulation

By far most commercial process simulators currently available are sequential modular process simulators. Each module contains the set of equations for that unit: the material and energy balances, equilibrium equations, physical property equations, and other internal unit equations. It calculates all output streams from input streams subject to module parameters. The stream variables commonly consist of component flows, temperature (or enthalpy) and pressure as the independent variables. Other dependent variables, such as total flow, vapor fraction, molecular weight and total enthalpy, are also available for each stream. The degrees of freedom for each module are used to specify conditions of the feed to the module, its operating conditions and module parameters. A typical process module is shown in Figure 4.1.

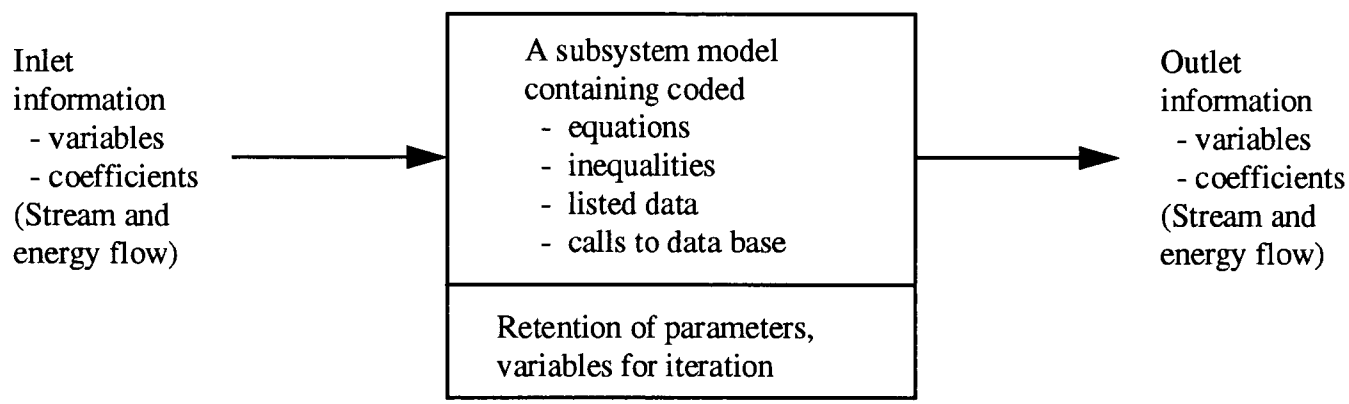

Figure 4.1 A typical process module showing the necessary interconnections of information

The task of a process simulator is to solve the equations for all modules in the process, and also the connectivity equations that relate the streams which pass from one module to another. The equations for an entire process can be written symbolically as:

$$\underline{h}(\underline{X}) = \underline{0} \qquad (4.1)$$

Where

$\underline{h}$ = Collection of all the process and connectivity equations

$\underline{X}$ = Process variables

In sequential modular process simulator, there are two major problems that seriously affect solution efficiency: recycle loops and design specifications. The problems caused by recycle loops are solved by introducing a "tear" stream for each loop (The stream variables of the tear stream are used as convergence criteria for the recycle loop.). Once the tear streams have been selected, the full set of equations is partitioned and then solved as sequential subsets. The solution of a simulation problem in a sequential modular process simulator is schematically shown in Figure 4.2.

In many simulation problems, dependent process variables that are calculated in the solution of the simulation problem (design specifications) must attain desired values. For example, it was necessary to be below a maximum dew point for sale gas in the natural gas problem. This kind of simulation problems is called the design problem or the constrained simulation problem.

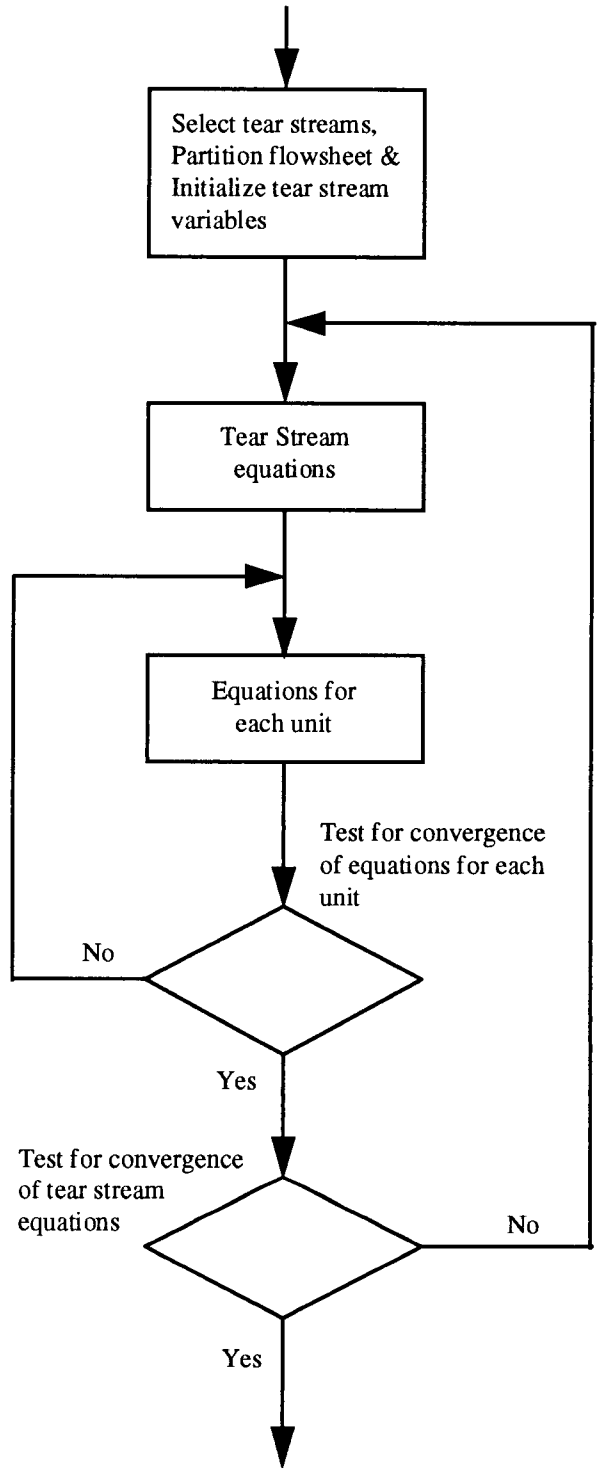

Figure 4.2 Schematic of a simulation problem in a sequential modular simulator

Mathematically, the equality design specifications can be expressed as:

$$\underline{c}(\underline{x},\underline{z}) = \underline{0} \tag{4.2}$$

where

$\underline{c}$ = Design specifications

$\underline{x}$ = Dependent process variables

$\underline{z}$ = Freed process variables

Note that process variables consists of dependent and freed (independent) variables, $\underline{X}$ = [$\underline{x}$, $\underline{z}$]. The freed variables, $\underline{z}$, can have arbitrary perturbations, while perturbations of the dependent variables, $\underline{x}$, must conform to process equations. The freed variables are so called "design" variables. The constrained simulation problem, then is to solve the system of equations:

$$\underline{h}(\underline{x},\underline{z}) = \underline{0} \tag{4.3}$$

$$\underline{c}(\underline{x},\underline{z}) = \underline{0}$$

$$\underline{g}(\underline{x},\underline{z}) \leq \underline{0}$$

where

$\underline{h}$ = Process equations

$\underline{c}$ = Equality design specifications

$\underline{g}$ = Inequalities representing the bounds imposed on the design variables or limits on design specifications

The bounds are allowed limits on the operating conditions. The final values of the design variables must be within the bounds for a feasible solution. This problem is generally handled by placing a root finding procedure (i.e., a single input-out put feedback control loop) around the modules and adjusting one parameter in a module for each design specification. For process with large interactions of design variables on design specifications, this single variable pairing strategy can be very ineffective. The solution of the constrained simulation problem is shown schematically in Figure 4.3

4.2 Optimization Using Process Simulators

Constrained simulation problems (the design problems) are often naturally posed as optimization problems (Gallier and Kisala, 1987). In a typical design problem, only practical upper and lower limits are known for the design variables. These variables provide the degrees of freedom for the optimization problem. Allowable limits for dependent variables form additional inequality constraints, while single value design specifications form the equality constraints. The engineering or economic objective function is defined in order to obtain maximum process profitability or efficiency. The objective function might be to maximize production rate or product purity, or to minimize byproduct formation or energy consumption. The process optimization problem can be stated as:

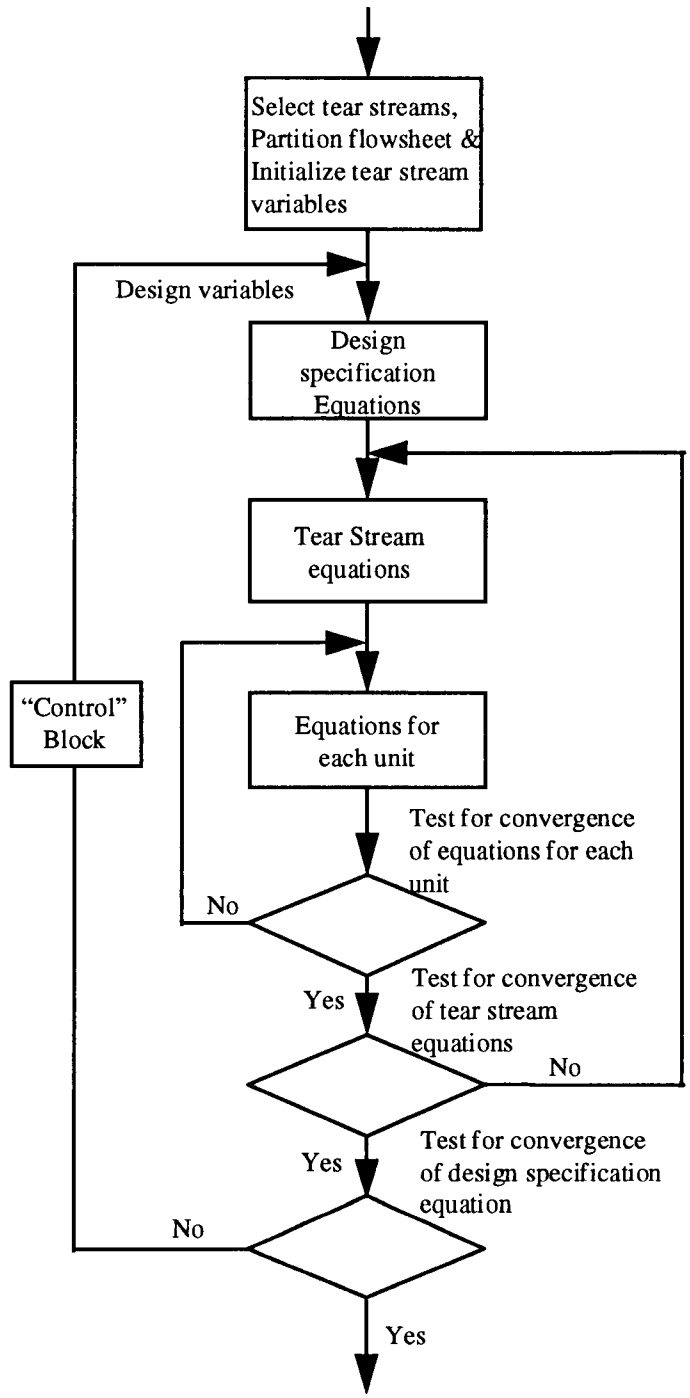

Figure 4.3 Schematic of a constrained simulation problem in a sequential modular simulator

$$\text{Maximize} \quad f(\underline{x},\underline{z}) \qquad \text{(equivalent to minimize } -f(\underline{x},\underline{z})) \qquad (4.4)$$

$$\text{Subject to} \quad \underline{h}(\underline{x},\underline{z}) = \underline{0}$$

$$\underline{c}(\underline{x},\underline{z}) = \underline{0}$$

$$\underline{g}(\underline{x},\underline{z}) \leq \underline{0}$$

where

f = Objective function

$\underline{h}$ = Process equations

$\underline{c}$ = Equality constraints

$\underline{g}$ = Inequality constraints

The early attempts to a combine process simulator with an optimization algorithm treated the process simulator as a "black box". Direct-search or random-search algorithms, which are *feasible path optimization* algorithms, have been used (Friedman and Pinder, 1976; Gaines and Gaddy, 1976; Ballman and Gaddy, 1977). These algorithms did not require derivatives of the objective function for optimization and information about the flowsheet was used in generating new guesses for the design variables. "Case study" approaches to optimization, similar to those of Chapter 3, also fall into this category. The black box optimization approach is shown schematically in Figure 4.4.

Although the feasible path optimizations using sequential process simulator are reasonably effective, they have difficulty in handling inequality constraints. Moreover, they are undesirable for solving large optimization problems since more than 100

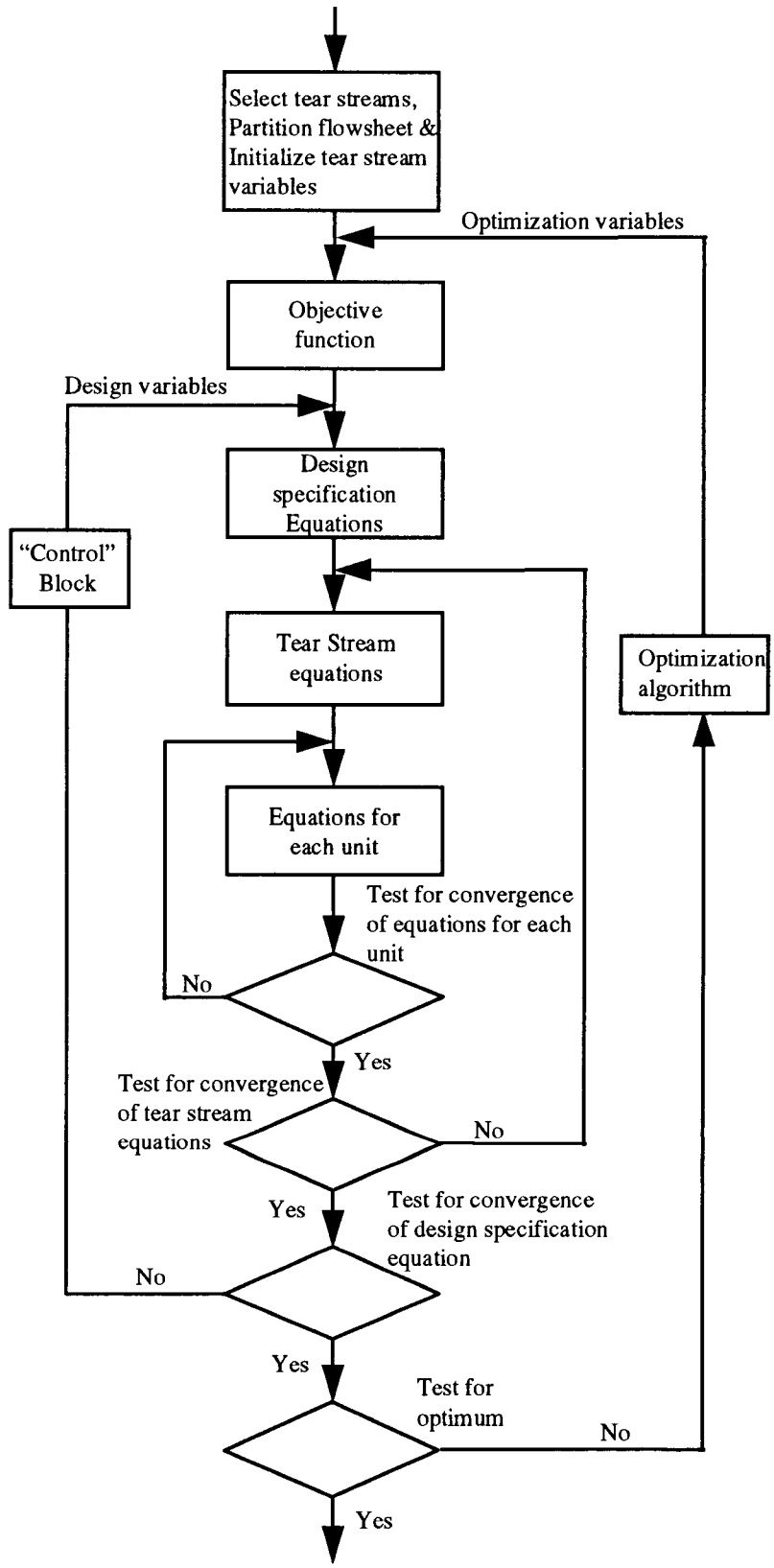

Figure 4.4 Black-box optimization

simulation time equivalents could be required (Ballman and Gaddy, 1977). A simulation time equivalent is the amount of computer time necessary to solve the optimization problem divided by the amount of time necessary to solve the simulation problem.

In developing Quadratic Approximation Programming (QAP), Parker and Hughes (1981) showed how to obtain gradient and other derivative information from a process simulator without resimulating the process for each perturbation. QAP was then modified by Biegler and Hughes (1981). The modified QAP was termed Quadratic/Linear Approximation Programming (Q/LAP) and used successive quadratic programming as its foundation. This method was shown to be more effective for process optimization using sequential modular simulators (Biegler and Hughes, 1982).

In this method, the optimization search automatically only converges on equalities as it approaches the optimum. For process optimization, this implies that the flowsheet equations only converge at the optimum. This concept of simultaneous convergence of process simulation and optimization was termed *infeasible path optimization.* As implied by its name, infeasible path optimization does not require the exact solution of each module on each pass through the simulator.

4.3 Successive Quadratic Programming

Successive quadratic programming (SQP) is an infeasible path optimization algorithm that handles nonlinear equality constraints, without requiring their convergence for each function evaluation and it is considered probably the most efficient general nonlinear programming (NLP) algorithms currently available. Berna, Locke and

Westerberg(1980) made the first application of this concept to chemical process simulation. At the heart of their algorithm is the successive quadratic programming method proposed by Powell(1977). Powell(1977), Schittkowski(1981), and Stadther et al.(1983) showed that SQP outperforms most of the other nonlinear programming algorithms. Also, Kisala, (1987) has shown that using SQP to solve process optimization problems can take fewer than 5 simulation time equivalents. The infeasible path algorithm is shown schematically in Figure 4.5. Because of SQP and other recent advances in nonlinear optimization, it is now possible to solve process optimization problems more efficiently (Biegler and Cuthrell, 1985).

The SQP algorithm minimizes a quadratic approximation of the Lagrangian function associated with the objective function and linear approximation of the constraints of the optimization problem. The resulting quadratic programming problem (QP) is formed using only one gradient and function evaluation from the nonlinear problem (gradient and derivative information are generally obtained from the process simulator by perturbation.). SQP converges by solving a QP at each iteration. The QP solution is then used as a search direction for the next step. A step size is chosen along this direction for which some merit function, measuring objective function improvement and constraint infeasibility, is minimized.

In this study, the natural gas process was optimized by using ASPEN PLUS, a sequential modular flow sheet simulator developed by Aspen Technology, Inc. ASPEN PLUS has an optimization capability that may be used to optimize a process by manipulating a feed stream and/or block input variables. Equality or inequality constraints

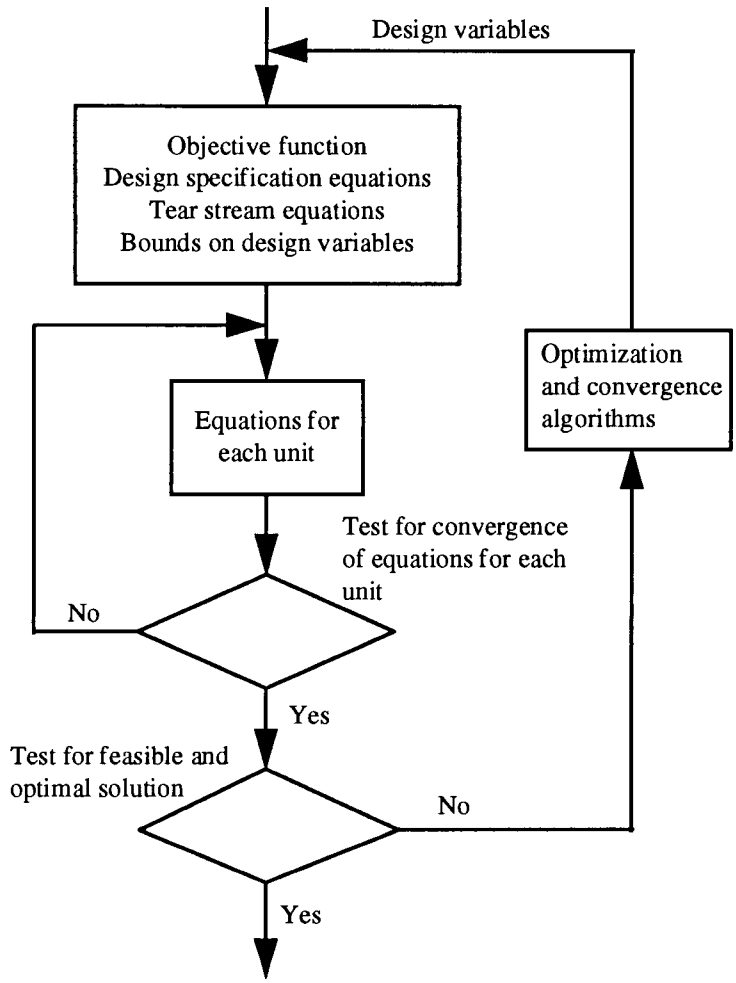

Figure 4.5 Infeasible path optimization

may be imposed on the optimization. The objective function and the constraint functions may be any flowsheet variables designated by the user or may be a function of flowsheet variables computed from user-written FORTRAN expressions. However, the actual details of the algorithm used are proprietary. For more details about SQP in general, *Optimization of Chemical Processes* by Edgar and Himmelblau (1981) is recommended for further reading.

Chapter 5

Results and Discussions

5.1 Nominal Design Conditions

In order to compare the differences between the two process simulators, the base case design of the natural gas process was simulated using CHEMCAD III and ASPEN PLUS. The specifications of feed stream and unit operations, thermodynamic property calculations, and convergence tolerances were set to be the same for both simulators. However, one difference in thermodynamic property calculations could not be made equivalent. CHEMCAD III has a specific calculation package, called Tri-Ethylene-Glycol/Water dehydration, which is not available in ASPEN PLUS. The thermodynamic calculation package in ASPEN PLUS, called Amines (Gas Sweetening), which gave the nearest results (considering flow rates and compositions of streams 25 and 26) was chosen. Process input and output streams obtained from both simulators are shown in Table 5.1.

It is obvious that the results from the two simulators are very close. Although for almost all calculations the same method of thermodynamic calculation was chosen for both simulators, some parameters or constants in the two packages were handled differently. For example, the vapor mole fraction of stream 5 calculated using ASPEN PLUS was about 2% higher than that calculated by CHEMCAD III, even though the temperature, pressure, flow rate and composition were the same.

Table 5.1 Comparison of process simulators used at nominal design condition

Stream Number	5		6	
	Feed to Inlet Separator		Condensate from Inlet Separator	
	CHEMCAD III	ASPEN PLUS	CHEMCAD III	ASPEN PLUS
Phase	Mixed	Mixed	Liquid	Liquid
Vapor Mole Fraction	0.851	0.869	0.000	0.000
Composition (Mol Frac)				
H_2O	0.1324*	0.1324*	0.0009	0.0007
CO_2	0.0912*	0.0912*	0.0316	0.0480
N_2	0.0022*	0.0022*	0.0001	0.0001
C_1	0.6130*	0.6130*	0.0859	0.0808
C_2	0.0837*	0.0837*	0.0571	0.0563
C_3	0.0390*	0.0390*	0.0829	0.0815
IC_4	0.0090*	0.0090*	0.0412	0.0405
NC_4	0.0094*	0.0094*	0.0588	0.0570
IC_5	0.0036*	0.0036*	0.0458	0.0448
NC_5	0.0027*	0.0027*	0.0417	0.0409
C_6	0.0028*	0.0028*	0.0828	0.0816
C_{7+}	0.0110*	0.0110*	0.4716	0.4676
TEG	0.0000*	0.0000*	0.0000	0.0000
Total (Mol%)	1.0000	1.0000	1.0000	1.0000
lbmols/hr	13025.00*	13025.00*	232.59	233.44
Temperature (F)	80.00*	80.00*	80.00	80.00
Pressure (psia)	315.00*	315.00*	315.00	315.00
Average MW	23.3990	23.3994	74.46	74.46

* Specified by user

Table 5.1 Comparison of process simulators used at nominal design condition (continued)

Stream Number	7		11	
	Water from Inlet Separator		Condensate from Suction Scrubber	
	CHEMCAD III	ASPEN PLUS	CHEMCAD III	ASPEN PLUS
Phase	Liquid	Liquid	Liquid	Liquid
Vapor Mole Fraction	0.000	0.000	0.000	0.000
Composition (Mol Frac)				
H_2O	1.0000	1.0000	N/A	0.0007
CO_2	0.0000	0.0000	N/A	0.0470
N_2	0.0000	0.0000	N/A	0.0001
C_1	0.0000	0.0000	N/A	0.0785
C_2	0.0000	0.0000	N/A	0.0552
C_3	0.0000	0.0000	N/A	0.0804
IC_4	0.0000	0.0000	N/A	0.0401
NC_4	0.0000	0.0000	N/A	0.0566
IC_5	0.0000	0.0000	N/A	0.0448
NC_5	0.0000	0.0000	N/A	0.0409
C_6	0.0000	0.0000	N/A	0.0821
C_{7+}	0.0000	0.0000	N/A	0.4734
TEG	0.0000	0.0000	N/A	0.0000
Total (Mol%)	1.0000	1.0000	N/A	1.0000
lbmols/hr	1704.94	1700.12	0.00	0.06
Temperature (F)	80.00	80.00	79.22	79.98
Pressure (psia)	315.00	315.00	305.00	305.00
Average MW	18.02	18.02	N/A	74.88

Table 5.1 Comparison of process simulators used at nominal design condition (continued)

Stream Number	25		26	
	Rich Glycol from Glycol Contactor		Lean Glycol to Glycol Contactor	
	CHEMCAD III	ASPEN PLUS	CHEMCAD III	ASPEN PLUS
Phase	Liquid	Liquid	Liquid	Liquid
Vapor Mole Fraction	0.000	0.000	0.000	0.000
Composition (Mol Frac)				
H_2O	0.2103	0.2500	0.0000*	0.0000*
CO_2	0.0453	0.0426	0.0000*	0.0000*
N_2	0.0000	0.0000	0.0000*	0.0000*
C_1	0.0359	0.0326	0.0000*	0.0000*
C_2	0.0222	0.0208	0.0000*	0.0000*
C_3	0.0199	0.0190	0.0000*	0.0000*
IC_4	0.0049	0.0048	0.0000*	0.0000*
NC_4	0.0086	0.0083	0.0000*	0.0000*
IC_5	0.0035	0.0034	0.0000*	0.0000*
NC_5	0.0031	0.0031	0.0000*	0.0000*
C_6	0.0026	0.0026	0.0000*	0.0000*
C_{7+}	0.0081	0.0083	0.0000*	0.0000*
TEG	0.6356	0.6044	1.0000*	1.0000*
Total (Mol%)	1.0000	1.0000	1.0000	1.0000
lbmols/hr	91.87	96.63	58.4*	58.4*
Temperature (F)	101.63	103.58	200.00*	200.00*
Pressure (psia)	990.00	990.00	1000.00*	1000.00*
Average MW	105.65	104.48	150.18	150.18

* Specified by user

Table 5.1 Comparison of process simulators used at nominal design condition (continued)

Stream Number	28		31	
	Condensate from Exp. Scrubber		Condensate from Cold Separator	
	CHEMCAD III	ASPEN PLUS	CHEMCAD III	ASPEN PLUS
Phase	Liquid	Liquid	Liquid	Liquid
Vapor Mole Fraction	0.000	0.000	0.000	0.000
Composition (Mol Frac)				
H_2O	0.0000	0.0000	0.0000	0.0000
CO_2	0.0822	0.1149	0.0818	0.1187
N_2	0.0004	0.0004	0.0004	0.0004
C_1	0.2778	0.2677	0.2517	0.2425
C_2	0.1247	0.1243	0.1315	0.1304
C_3	0.1340	0.1323	0.1559	0.1527
IC_4	0.0526	0.0519	0.0641	0.0627
NC_4	0.0681	0.0664	0.0836	0.0808
IC_5	0.0405	0.0393	0.0493	0.0471
NC_5	0.0337	0.0326	0.0403	0.0384
C_6	0.0443	0.0410	0.0441	0.0402
C_{7+}	0.1417	0.1289	0.0971	0.0860
TEG	0.0000	0.0000	0.0000	0.0000
Total (Mol%)	1.0000	1.0000	1.0000	1.0000
lbmols/hr	104.15	129.43	120.93	126.25
Temperature (F)	69.86	70.66	50.24	51.61
Pressure (psia)	975.00	975.00	800.00	800.00
Average MW	48.13	47.46	47.07	46.37

Table 5.1 Comparison of process simulators used at nominal design condition (continued)

Stream Number	161		41	
	Condensate from Sale Gas Sep.		Sale gas	
	CHEMCAD III	ASPEN PLUS	CHEMCAD III	ASPEN PLUS
Phase	Liquid	Liquid	Vapor	Vapor
Vapor Mole Fraction	0.000	0.000	1.000	1.000
Composition (Mol Frac)				
H_2O	N/A	N/A	0.0000	0.0000
CO_2	N/A	N/A	0.1069	0.1058
N_2	N/A	N/A	0.0026	0.0026
C_1	N/A	N/A	0.7297	0.7313
C_2	N/A	N/A	0.0966	0.0965
C_3	N/A	N/A	0.0419	0.0417
IC_4	N/A	N/A	0.0087	0.0086
NC_4	N/A	N/A	0.0084	0.0083
IC_5	N/A	N/A	0.0024	0.0023
NC_5	N/A	N/A	0.0016	0.0015
C_6	N/A	N/A	0.0006	0.0006
C_{7+}	N/A	N/A	0.0006	0.0005
TEG	N/A	N/A	0.0000	0.0000
Total (Mol%)	N/A	N/A	1.0000	1.0000
lbmols/hr	0.00	0.00	10828.92	10797.00
Temperature (F)	106.91	112.50	127.16	122.27
Pressure (psia)	876.00	875.00	1330.00	1330.00
Average MW	N/A	N/A	22.63	22.57

Another possibility for differences is the pure component data bases in the two simulators. The physical properties would be another source of differences, but this should be relatively insignificant. For example, with the same specification of components, molecular weights of stream 5 calculated by CHEMCAD III and ASPEN PLUS are different, but only in the fourth decimal position.

Differences of parameters in unit operation modules could also lead to the differences in results. As an example, consider the Inlet Separator, where the input stream was stream 5 and output streams were streams 6 and 7. In this unit, an isothermal flash calculation was specified for both CHEMCAD III and ASPEN PLUS. With the same specifications of input variables, stream and block variables, the results in output streams from the two simulators were different, i.e. flow rates of stream 6 and 7 calculated using ASPEN PLUS were respectively about 0.4% higher and 0.3% lower than those calculated by CHEMCAD III. Other possibilities for differences in results are system convergence specifications, numerical formats, etc., although the differences caused by these possibilities are difficult to identify.

The economic objective function at nominal design conditions was calculated using output information from each of the two simulators. As shown in Table 5.2, the biggest difference was condensate sale. The condensate sale calculated using ASPEN PLUS was about 7% higher than that calculated using CHEMCAD III. This was a direct result of using different thermodynamic calculations in the Glycol Contactor. However, total sales were within 1% of each other. Thus, the results from the two simulators are close enough

that from an engineering point of view, the results can be considered equivalent for process design work.

Table 5.2 Comparison of yields at nominal design conditions

Simulator Used	Gas Sale (US$/day)	Condensate Sale (US$/day)	Total Sales (US$/day)
CHEMCAD III	386,878.36	95,183.21	482,061.57
ASPEN PLUS	384,664.33	101,926.89	486,591.22

5.2 Global Objective Model

The experimental results from the global approximation approach are shown in Table 5.3. The second-order polynomial approximation model was obtained using the method of least squares as given by the formulae in Tables 3.4 and 3.5. The empirical model obtained was;

$$y = \beta_0 + \sum_{i=1}^{7} \beta_i x_i + \sum_{i=1}^{7} \beta_{ii} x_i^2 + \sum_{\substack{i=1 \\ i<j}}^{7} \sum_{j=1}^{7} \beta_{ij} x_i x_j \qquad (5.1)$$

Analysis of variance for the approximation, and numerical values of the β s and their standard errors are given in Tables 5.4 and 5.5, respectively. R-square value for the model fitting was 0.9992, indicating a good fit by the model. Note that the simulation results for the nominal design, run #57 to #62, are slightly different. This is because of the difference

Table 5.3 Experimental Results

No.	x_1	x_2	x_3	x_4	x_5	x_6	x_7	YIELD
1	0	0	0	+1	+1	+1	0	479,329.74
2	0	0	0	+1	+1	-1	0	501,850.74
3	0	0	0	+1	-1	+1	0	478,510.35
4	0	0	0	+1	-1	-1	0	501,695.83
5	0	0	0	-1	+1	+1	0	466,217.93
6	0	0	0	-1	+1	-1	0	483,392.98
7	0	0	0	-1	-1	+1	0	465,543.57
8	0	0	0	-1	-1	-1	0	483,354.16
9	+1	0	0	0	0	+1	+1	474,308.52
10	+1	0	0	0	0	+1	-1	473,524.69
11	+1	0	0	0	0	-1	+1	493,466.59
12	+1	0	0	0	0	-1	-1	492,996.63
13	-1	0	0	0	0	+1	+1	472,571.35
14	-1	0	0	0	0	+1	-1	471,808.93
15	-1	0	0	0	0	-1	+1	493,927.65
16	-1	0	0	0	0	-1	-1	493,372.29
17	0	+1	0	0	+1	0	+1	483,366.15
18	0	+1	0	0	+1	0	-1	482,786.36
19	0	+1	0	0	-1	0	+1	483,018.20
20	0	+1	0	0	-1	0	-1	482,444.52
21	0	-1	0	0	+1	0	+1	482,356.14
22	0	-1	0	0	+1	0	-1	481,711.57
23	0	-1	0	0	-1	0	+1	481,962.52
24	0	-1	0	0	-1	0	-1	481,293.36
25	+1	+1	0	+1	0	0	0	489,987.22
26	+1	+1	0	-1	0	0	0	474,973.55
27	+1	-1	0	+1	0	0	0	488,968.70
28	+1	-1	0	-1	0	0	0	474,116.97
29	-1	+1	0	+1	0	0	0	489,398.55
30	-1	+1	0	-1	0	0	0	474,573.09
31	-1	-1	0	+1	0	0	0	488,048.77
32	-1	-1	0	-1	0	0	0	473,496.52
33	0	0	+1	+1	0	0	+1	479,712.09
34	0	0	+1	+1	0	0	-1	478,984.54
35	0	0	+1	-1	0	0	+1	467,581.06
36	0	0	+1	-1	0	0	-1	466,934.47
37	0	0	-1	+1	0	0	+1	502,131.54
38	0	0	-1	+1	0	0	-1	501,340.37
39	0	0	-1	-1	0	0	+1	482,717.25
40	0	0	-1	-1	0	0	-1	481,344.13
41	+1	0	+1	0	+1	0	0	475,210.48
42	+1	0	+1	0	-1	0	0	474,831.83
43	+1	0	-1	0	+1	0	0	493,729.48
44	+1	0	-1	0	-1	0	0	493,368.10
45	-1	0	+1	0	+1	0	0	473,771.12
46	-1	0	+1	0	-1	0	0	473,272.60
47	-1	0	-1	0	+1	0	0	493,030.71
48	-1	0	-1	0	-1	0	0	492,653.05
49	0	+1	+1	0	0	+1	0	465,093.49
50	0	+1	+1	0	0	-1	0	484,932.98
51	0	+1	-1	0	0	+1	0	485,010.34
52	0	+1	-1	0	0	-1	0	504,529.01
53	**0**	**-1**	**+1**	**0**	**0**	**+1**	**0**	**462,160.03**
54	0	-1	+1	0	0	-1	0	484,463.34
55	0	-1	-1	0	0	+1	0	483,345.70
56	**0**	**-1**	**-1**	**0**	**0**	**-1**	**0**	**504,698.76**
57	0	0	0	0	0	0	0	482,420.15
58	0	0	0	0	0	0	0	482,428.45
59	0	0	0	0	0	0	0	482,463.81
60	0	0	0	0	0	0	0	482,277.91
61	0	0	0	0	0	0	0	482,388.85
62	0	0	0	0	0	0	0	482,425.08

Table 5.4 Analysis of Variance

	Sum of Squares	D.F.	Mean Squares	F-Ration	P-Value
Linear Terms					
x_1	3.8065×10^6	1	3.8065×10^6	18.08	0.0003
x_2	7.5837×10^6	1	7.5837×10^6	36.02	0.0000
x_3	2.2224×10^9	1	2.2224×10^9	10555.34	0.0000
x_4	1.4371×10^9	1	1.4371×10^9	6825.24	0.0000
x_5	9.6213×10^5	1	9.6213×10^5	4.57	0.0425
x_6	2.5063×10^9	1	2.5063×10^9	11903.51	0.0000
x_7	3.0654×10^6	1	3.0654×10^6	14.56	0.0008
Interaction Terms					
x_1x_2	3.7985×10^4	1	3.7985×10^4	0.18	0.6792
x_1x_3	3.1394×10^5	1	3.1394×10^5	1.49	0.2334
x_1x_4	2.9730×10^4	1	2.9730×10^4	0.14	0.7142
x_1x_5	2.3171×10^3	1	2.3171×10^3	0.01	0.9184
x_1x_6	2.3001×10^6	1	2.3001×10^6	10.92	0.0029
x_1x_7	5.1184×10^2	1	5.1184×10^2	0.00	0.9616
x_2x_3	4.5516×10^5	1	4.5516×10^5	2.16	0.1540
x_2x_4	2.3669×10^4	1	2.3669×10^4	0.11	0.7438
x_2x_5	1.8617×10^3	1	1.8617×10^3	0.01	0.9268
x_2x_6	2.3093×10^6	1	2.3093×10^6	10.97	0.0028
x_2x_7	3.2104×10^3	1	3.2104×10^3	0.02	0.9040
x_3x_4	2.8992×10^7	1	2.8992×10^7	137.70	0.0000
x_3x_5	2.3850×10^3	1	2.3850×10^3	0.01	0.9172
x_3x_6	2.0195×10^5	1	2.0195×10^5	0.96	0.3471
x_3x_7	7.8042×10^4	1	7.8042×10^4	0.37	0.5546
x_4x_5	8.5230×10^3	1	8.5230×10^3	0.04	0.8443
x_4x_6	1.4367×10^7	1	1.4367×10^7	68.24	0.0000
x_4x_7	3.1374×10^4	1	3.1374×10^4	0.15	0.7068
x_5x_6	2.1126×10^5	1	2.1126×10^5	1.00	0.3261
x_5x_7	4.2689×10^1	1	4.2689×10^1	0.00	0.9889
x_6x_7	3.3921×10^4	1	3.3921×10^4	0.16	0.6958
Quadratic Terms					
x_1^2	2.5448×10^5	1	2.5448×10^5	1.21	0.2821
x_2^2	1.1889×10^4	1	1.1889×10^4	0.06	0.8166
x_3^2	1.6402×10^7	1	1.6402×10^7	77.90	0.0000
x_4^2	8.9211×10^6	1	8.9211×10^6	42.37	0.0000
x_5^2	1.1721×10^5	1	1.1721×10^5	0.56	0.4705
x_6^2	8.7687×10^6	1	8.7687×10^6	41.65	0.0000
x_7^2	1.2665×10^5	1	1.2665×10^5	0.60	0.4535
Block	1.6891×10^4	1	1.6891×10^4	0.60	0.4535
Residual	5.2637×10^6	25	2.1055×10^5		
Total	6.2750×10^9	61			

Table 5.5 The global RSM model's coefficients and standard errors

Constant	Linear Terms	Quadratic Terms	Interaction Terms	
β_0 : 482401.00	β_1 : 398.26	β_{11} : 137.30	β_{12} : -68.91	β_{34} : -1903.68
	β_2 : 562.13	β_{22} : -29.68	β_{13} : 198.10	β_{35} : 17.27
	β_3 : -9622.93	β_{33} : 1102.24	β_{14} : 60.96	β_{36} : -158.88
	β_4 : 7738.03	β_{44} : -812.91	β_{15} : -17.02	β_{37} : -98.77
	β_5 : 200.22	β_{55} : 93.18	β_{16} : 536.21	β_{45} : 32.64
	β_6 : -10,219.00	β_{66} : 805.94	β_{17} : -8.00	β_{46} : -1340.11
	β_7 : 357.38	β_{77} : -96.86	β_{23} : 238.53	β_{47} : -62.62
			β_{24} : 54.39	β_{56} : 162.50
			β_{25} : -15.26	β_{57} : -2.31
			β_{26} : 537.28	β_{67} : 65.12
			β_{27} : -20.03	
std. err = 187.33	std. err = 93.66	std. err = 162.23	std. err = 112.57	

Table 5.6 Sensitivity analysis of the global RSM model

	Yield at each manipulated x_i (x 10^5 US$/day)						
	x_1	x_2	x_3	x_4	x_5	x_6	x_7
Maximum	4.8294	4.8293	4.9313	4.8933	4.8269	4.9343	4.8266
Minimum	4.8214	4.8181	4.7388	4.7388	4.8229	4.7299	4.8195
Difference (%)	0.1660	0.2323	3.9933	3.2050	0.0830	4.2401	0.1473

in initial values of tear stream variables. As order of simulation runs was randomized, the initial values of the tear stream variables for each run were, therefore, different because they were "held" from previous simulation run.

From the empirical model, sensitivity analyses were performed. Each decision variable was varied from -1 to +1 while keeping the others at nominal design conditions. Three decision variables (x_3, x_4 and x_6) were found to have relatively significant effects on the response variable (y). However, the effects of those three variables are small with maximum differences were less than 5%. The sensitivity analysis results are given in Table 5.6, and graphically shown in Figures 5.1-5.7.

The empirical model (the global RSM model) was then optimized using an SQP algorithm. The initial design for this optimization problem was the nominal design, [x_1, x_2, x_3,x_4,x_5,x_6,x_7] = [0,0,0,0,0,0,0]. The result optimal design was [x_1, x_2, x_3,x_4,x_5,x_6,x_7] = [-1,-1,-1,1,1,-1,1]. The optimization results from this approach are shown in Table 5.7.

Table 5.7 Optimization result from global approximation approach (evaluated using CHEMCAD III)

Conditions	Gas Sale (US$/day)	Condensate Sale (US$/day)	Total Sale (US$/day)
Nominal design condition	387,150.77	95,250.23	482,401.00
Optimum condition	361,972.82	153,097.23	515,070.05

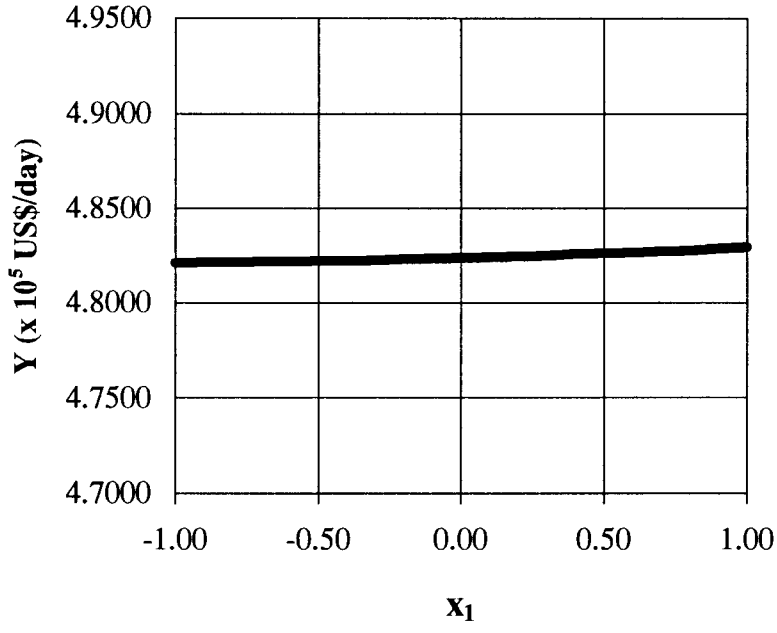

Figure 5.1 Sensitivity analysis of the global RSM model: effect of x_1

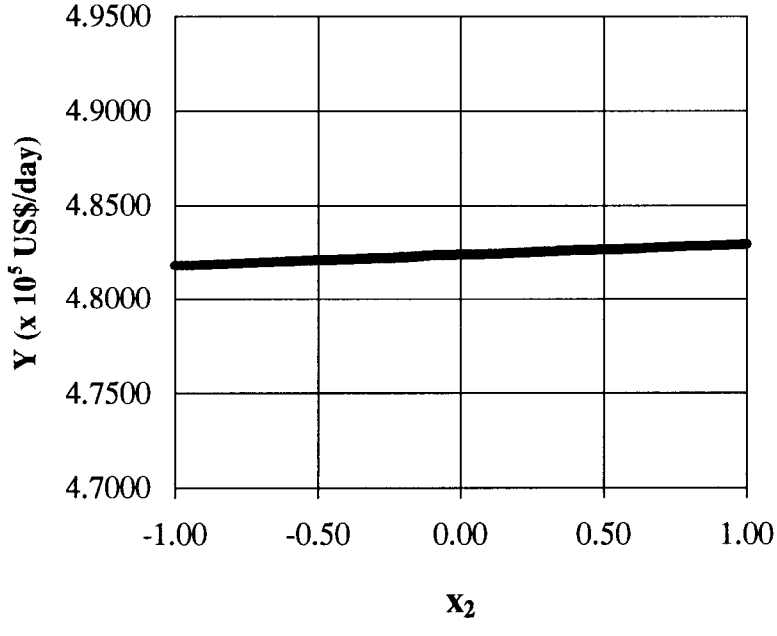

Figure 5.2 Sensitivity analysis of the global RSM model: effect of x_2

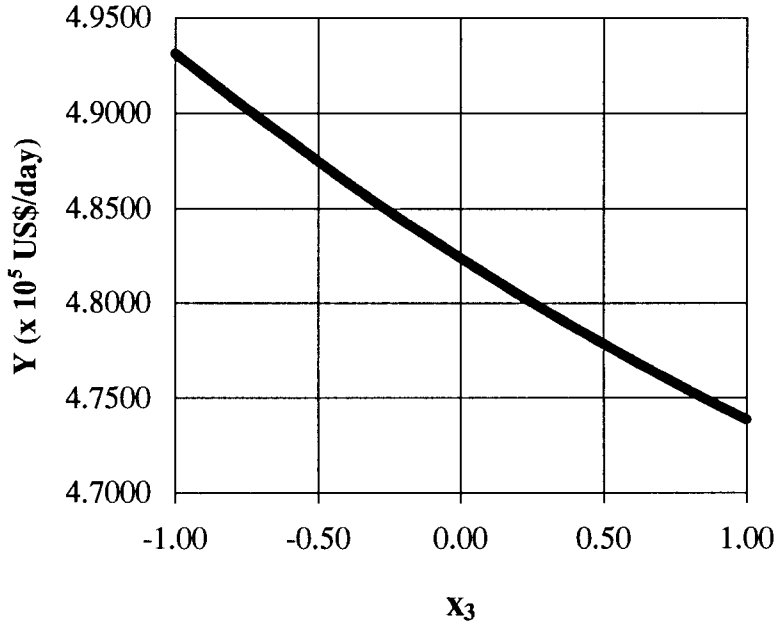

Figure 5.3 Sensitivity analysis of the global RSM model: effect of x_3

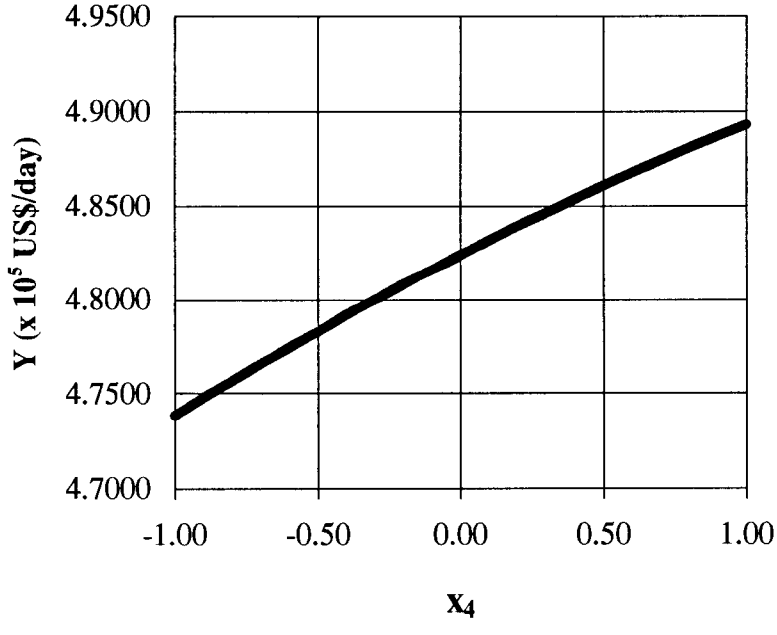

Figure 5.4 Sensitivity analysis of the global RSM model: effect of x_4

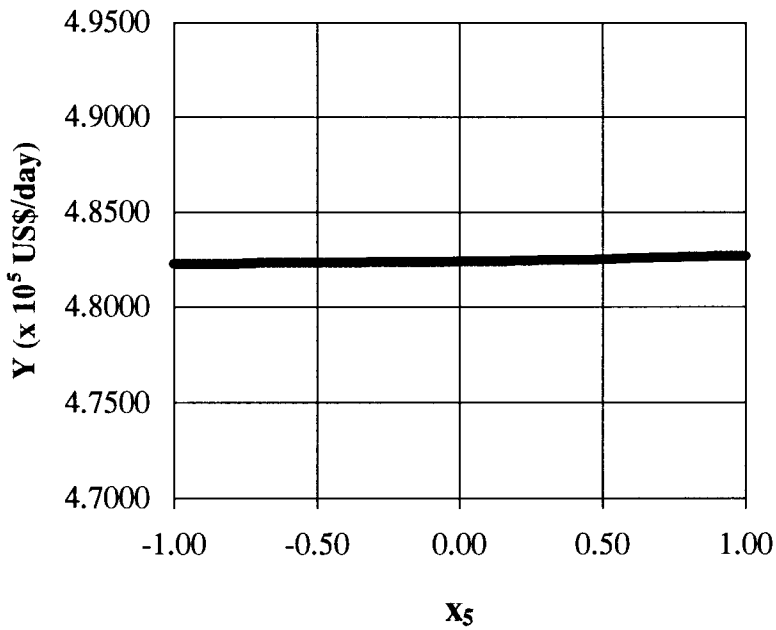

Figure 5.5 Sensitivity analysis of the global RSM model: effect of x_5

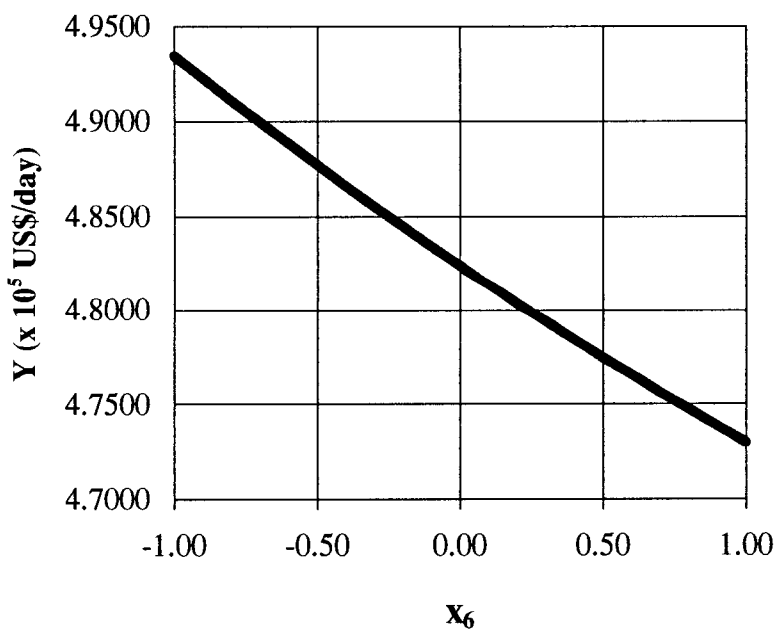

Figure 5.6 Sensitivity analysis of the global RSM model: effect of x_6

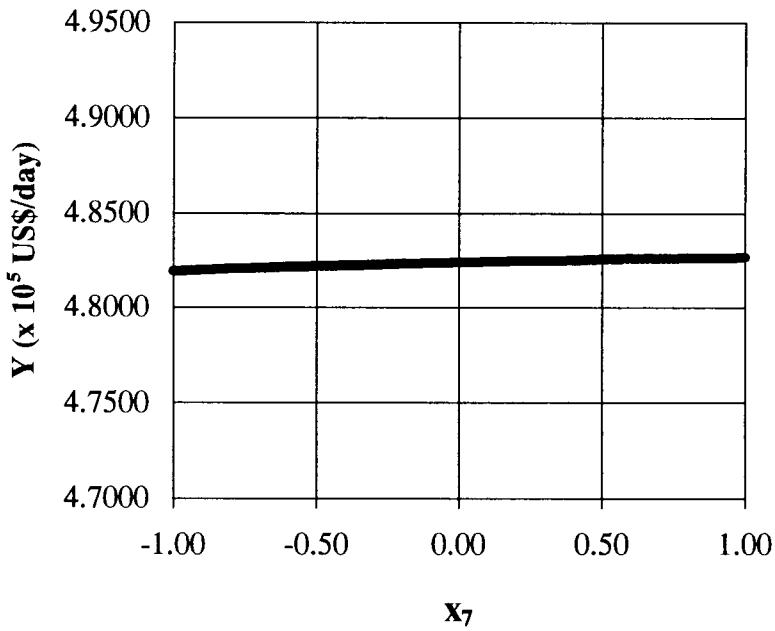

Figure 5.7 Sensitivity analysis of the global RSM model: effect of x_7

From the optimization results and sensitivity analysis of the model, it is seen that the response model is quite flat. The difference between the maximum and minimum yields obtained as case examples was just 8.8%. The optimal yield was only 6.9% higher than the nominal yield, and only 2.2% greater than the "best" case evaluated in the experimental design. Optimization results from the global approximation and "case study" approaches are shown in Table 5.8. However, if the numbering of the design variables were different, a slightly different quadratic model would be obtained and the global optimum might be acquired directly from one of the simulations. For example, if the order of xs is changed to $[x_1, x_2, x_5, x_3, x_6\ x_4, x_7]$, the global optimum would be obtained directly from simulation #7 (see Table 5.3).

Table 5.8 Comparison of optimization results from "case study" and global RSM model approaches

Conditions	Decision Variables							Yield (US$/day)
	x_1	x_2	x_3	x_4	x_5	x_6	x_7	
Nominal design	0	0	0	0	0	0	0	482,401.00
Best of case studies (# 56)	0	-1	-1	0	0	-1	0	504,698.76
Optimum from global RSM model	-1	-1	-1	1	1	-1	1	515,070.05

Note that if only the three variables which have significant effects on the objective function had been chosen as design variables, the number of simulations required would have been lowered to 15 runs, compared to 62 runs for the 7-factor design. This could have reduced the time spent in simulation, while having an equivalent optimization result. The optimal objective value obtained from a "reduced" RSM model (reset $x_1 = x_2 = x_5 = x_7 = 0$) was 514,161.14 US$/day, about 0.3% lower than the optimal objective value obtained from the global RSM model.

At the optimum, all design variables were at one of their boundaries. Pressure drops across the Inlet Separator and the Compressor Scrubber, and the compression ratio of the Production Compressor and the Expander were at their lower limits, while the pressure drop across the Expander Scrubber and Cold separator, and the heat duty of Gas/Gas Exchanger are at their upper limits.

Since the natural gas process has two products, condensate and sale gas, the optimal operating conditions reflect a trade-off between these two products to yield

maximum total sales. This trade-off depends on unit prices of both sale gas and raw condensate, with the unit prices behaving as weighting constants in the objective function. In this study, unit prices of sale gas and raw condensate were fixed at 3.60 US$/mmbtu (gross) and 5.24 US$/ft^3 (std) respectively.

From the optimization results, increased production of condensate appeared to be the means of increasing total sales above the nominal design's result. A lower compression ratio for the production compressor (v_3) increase the condensation of gas in the Expander Scrubber, since both pressure and temperature were lowered. A higher heat exchange rate for the Gas/Gas Exchanger cools the feed to the Expander Scrubber and increases the condensation. A lower compression ratio (< 1) for the Expander results in lower pressure and temperature in the Cold Separator and more condensate formation.

5.3 SQP Results with ASPEN PLUS

In this approach, the natural gas processing plant was simulated and optimized using ASPEN PLUS. Two optimization searches from two different initial designs were performed. The initial designs used in this approach were 1) nominal design condition, $[x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [0,0,0,0,0,0,0]$, and 2) close to the optimum of the global RSM model $[x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [-0.8,-0.8,-0.8,0.8,0.8,-0.8,0.8]$. Both optimization searches converged in two iterations. Table 5.9 shows the total sales results from both searches. The optimal design variables of the two optimization searches and nominal design case using ASPEN PLUS are compared in Table 5.10 and the histories of the searches for the optimum design conditions are shown in Table 5.11.

The optimization results show that the final design for this approach depended on the initial design, although total sales of both final design were very close. The difference between total sales of case #1 and case #2 was just 0.05%. The criterion used to terminate calculations was a stationary condition of the associated Lagrangian function. The Lagrangian tolerance , ε , was specified as 0.0001. This was the smallest tolerance that the optimization searches converged.

As shown in Table 5.10, the decision variables x_3, x_4 and x_6 converged to the same points, no matter what the initial condition was. On the other hand, the final values of decision variables x_1, x_2, x_5 and x_7 were very close to their initial values. Sensitivity analyses of the ASPEN PLUS model are reported in Table 5.12, and graphically shown in Figures 5.8 to 5.14, along with results from CHEMCAD III. Although the objective function evaluations were slightly different for the two simulators, the nearly parallel curves in these figures indicate that the simulators predict similar directions for objective improvement. As could be expected from the sensitivities, the final designs of case #1 and case #2 are different only in those design variables which have little influence on the objective. Physical explanations for the effects of the main design variables were discussed in section 5.2.

Table 5.9 Optimization result from successive quadratic approximation approach: using ASPEN PLUS

Conditions	Gas Sale (US$/day)	Condensate Sale (US$/day)	Total Sale (US$/day)
Nominal design condition	384,664.33	101,926.89	486,591.22
Optimum condition: case# 1	360,403.73	161,893.86	522,297.59
Optimum condition: case# 2	360,443.10	162,133.05	522,576.15

Note : Case# 1-Initial condition = [0,0,0,0,0,0,0].
Case# 2-Initial condition = [-0.8,-0.8,-0.8,0.8,0.8,-0.8,0.8].

Table 5.10 Comparison of the optimization results using ASPEN PLUS

Conditions	Decision Variables							Yield (US$/day)
	x_1	x_2	x_3	x_4	x_5	x_6	x_7	
Nominal design	0	0	0	0	0	0	0	486,591.22
Final ASPEN design: case#1	0	0	-1	0.8	0	-1	0	522,297.59
Final ASPEN design: case#2	-0.8	-0.8	-1	0.8	0.8	-1	0.8	522,576.15

Note : Case# 1-Initial condition = [0,0,0,0,0,0,0].
Case# 2-Initial condition = [-0.8,-0.8,-0.8,0.8,0.8,-0.8,0.8].

Table 5.11 History of the optimization searches using ASPEN PLUS

Case# 1 : Initial condition = [0,0,0,0,0,0,0]									
Iteration No.	Objective Function	Lagrangian Function	x_1	x_2	x_3	x_4	x_5	x_6	x_7
0	4.8659E5	Missing	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1	5.2230E5	5.2230E5	0.01	0.03	-1.00	0.80	0.01	-1.00	0.01
2	5.2230E5	5.2229E5	0.01	0.03	-1.00	0.80	0.01	-1.00	0.01
Case# 2 : Initial condition = [-0.8,-0.8,-0.8,0.8,0.8,-0.8,0.8]									
Iteration No.	Objective Function	Lagrangian Function	x_1	x_2	x_3	x_4	x_5	x_6	x_7
0	5.1596E5	Missing	-0.80	-0.80	-0.80	0.80	0.80	-0.80	0.80
1	5.2258E5	5.2255E5	-0.80	-0.78	-1.00	0.80	0.81	-1.00	0.80
2	5.2258E5	5.2254E5	-0.80	-0.78	-1.00	0.80	0.81	-1.00	0.80

Table 5.12 Sensitivity analysis of the simulation model (ASPEN PLUS)

	Yield at each manipulated x_i (x 10^5 US$/day)						
	x_1	x_2	x_3	x_4	x_5	x_6	x_7
Maximum	4.8699	4.8727	5.0003	4.9320	4.8680	4.9920	4.8695
Minimum	4.8609	4.8580	4.7646	4.7630	4.8635	4.7621	4.8619
Difference (%)	0.1850	0.3021	4.8439	3.4731	0.0925	4.7247	0.1562
RSM Diff. (%)	0.1660	0.2323	3.9933	3.2050	0.0830	4.2401	0.1473

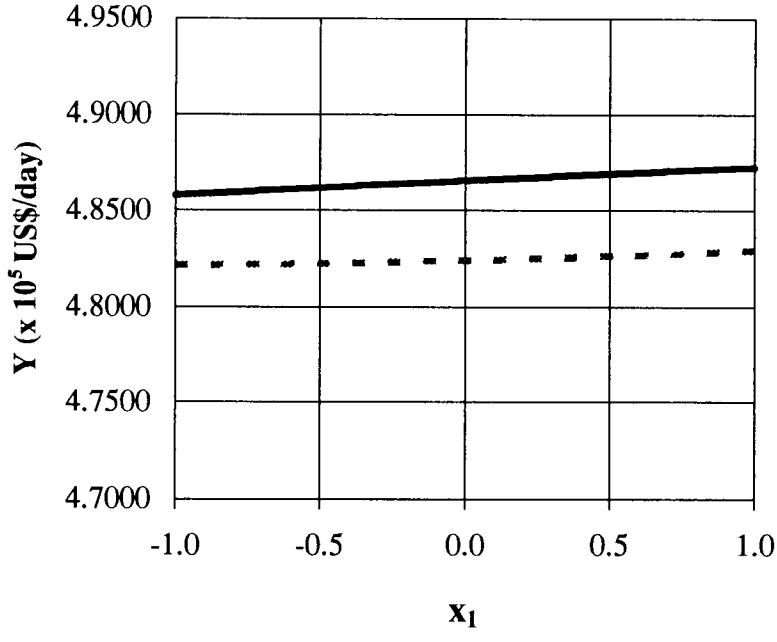

Figure 5.8 Sensitivity analysis of the simulation models: effect of x_1 (solid = ASPEN PLUS, dashed = CHEMCAD III)

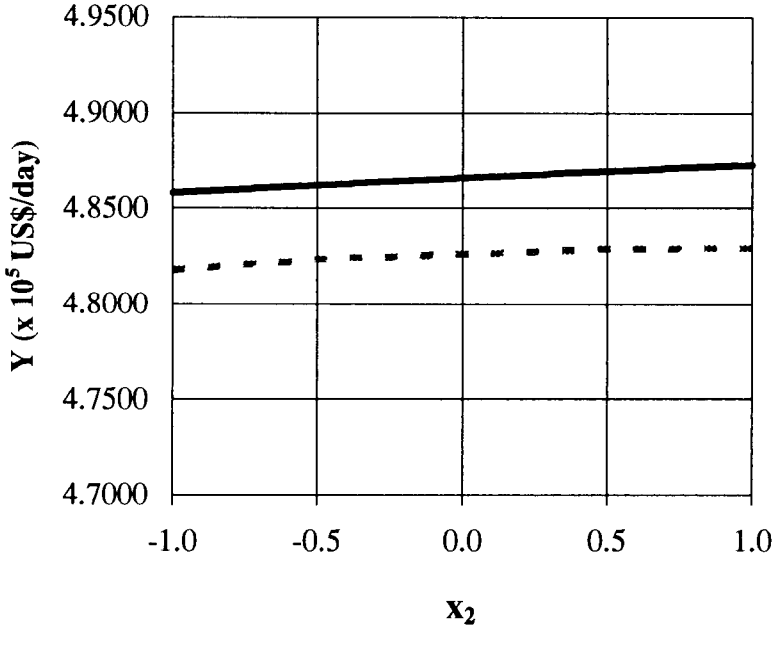

Figure 5.9 Sensitivity analysis of the simulation models: effect of x_2 (solid = ASPEN PLUS, dashed = CHEMCAD III)

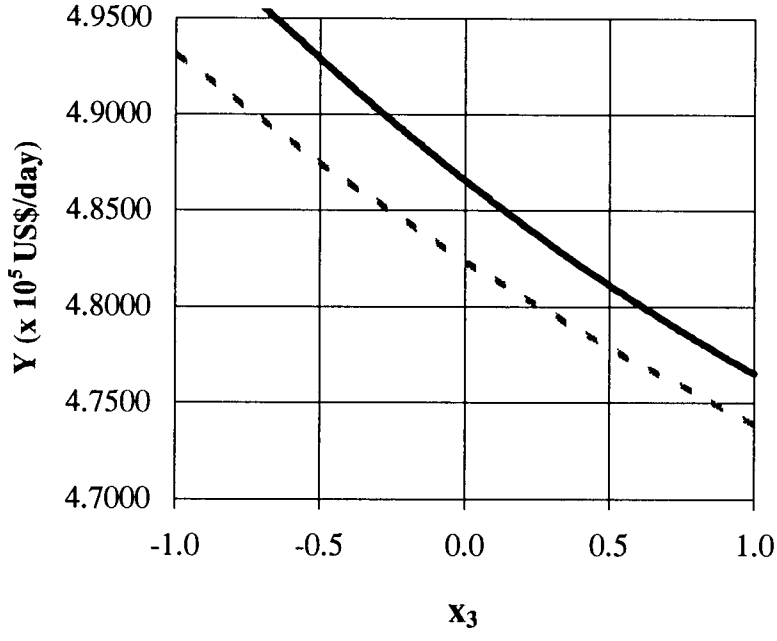

Figure 5.10 Sensitivity analysis of the simulation models: effect of x_3 (solid = ASPEN PLUS, dashed = CHEMCAD III)

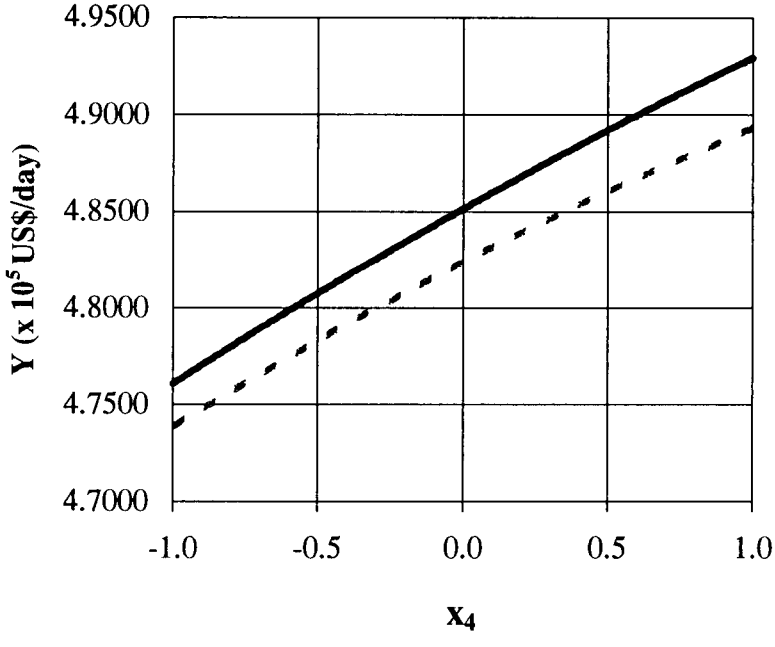

Figure 5.11 Sensitivity analysis of the simulation models: effect of x_4 (solid = ASPEN PLUS, dashed = CHEMCAD III)

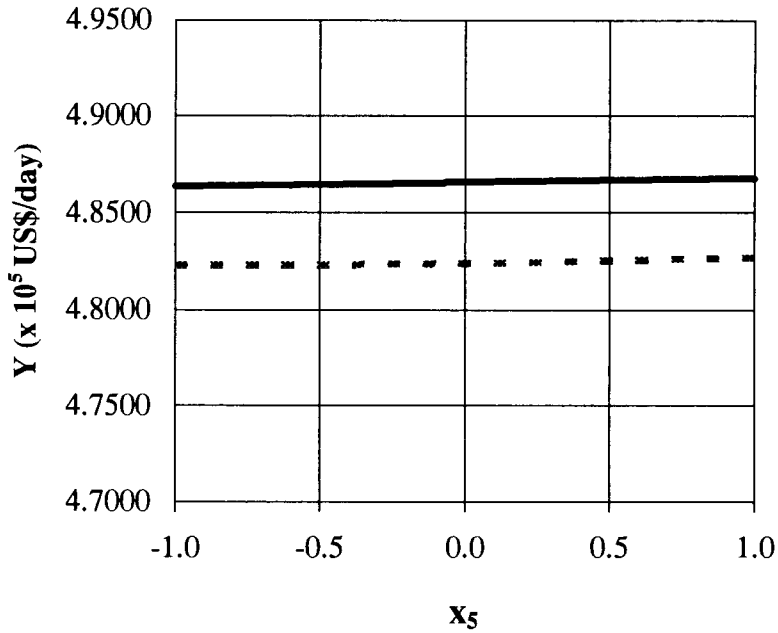

Figure 5.12 Sensitivity analysis of the simulation models: effect of x_5 (solid = ASPEN PLUS, dashed = CHEMCAD III)

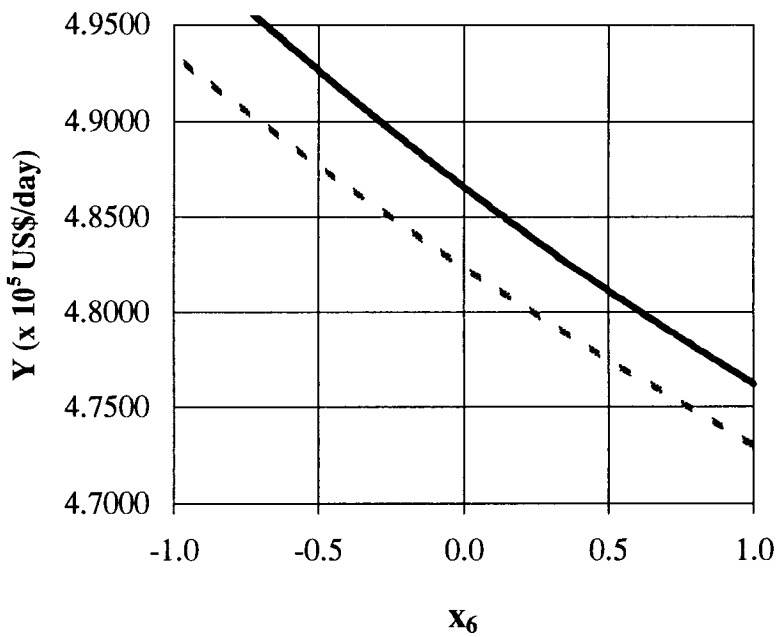

Figure 5.13 Sensitivity analysis of the simulation models: effect of x_6 (solid = ASPEN PLUS, dashed = CHEMCAD III)

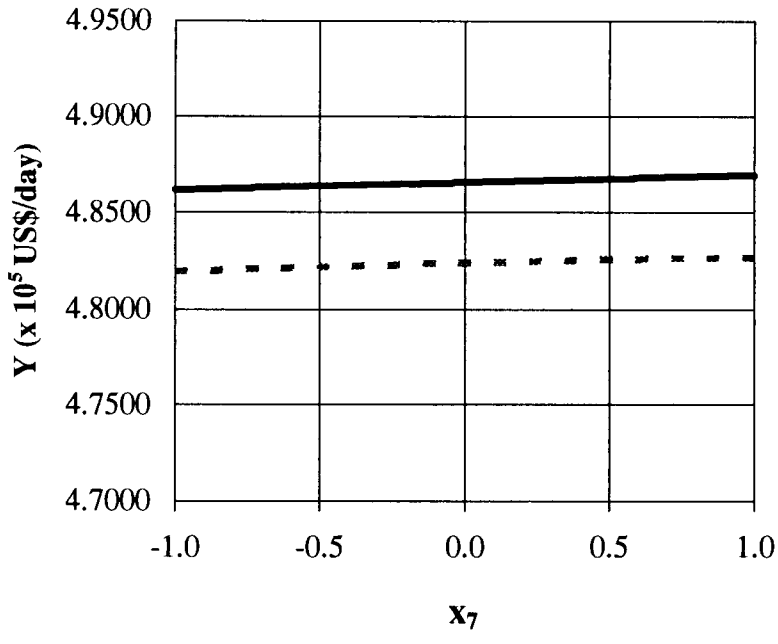

Figure 5.14 Sensitivity analysis of the simulation models: effect of x_7 (solid = ASPEN PLUS, dashed = CHEMCAD III)

5.4 Comparison of Optimization Results from Alternative Approaches

The maximum objective value from the two approaches are close, even though the design variables are somewhat different. This is because the variables that make the combinations different do not have substantial effects on yield. In order to compare the results equitably, the optimal design variables obtained from the RSM model and the modeling experiments were used in ASPEN PLUS simulations and the results are shown in Table 5.13, along with the final designs found using the SQP capability of ASPEN PLUS.

The global optimal conditions for this problem were at design variable limits, but only the global approximation approach identified that design. However, the differences

between the yields at the final designs found with the local approach versus the global approach were very small, 0.29 and 0.23% for case# 1 and case# 2, respectively when designs were simulated using ASPEN PLUS.

Yields from the simulation model using CHEMCAD, the global RSM model and using ASPEN PLUS are given in Table 5.14. The global RSM model predicts the correlation between design variables and the objective function very well. Yields calculated using the global RSM model at nominal design and optimal conditions are very close to yields obtained by using CHEMCAD III, as expected for the Box-Behnken design. Moreover, results of sensitivity analysis of the RSM model gave comparable results to those of the ASPEN PLUS simulation model.

Referring to Kuhn-Tucker (KT) necessary optimality criteria for a constrained optimization problem (Kuhn and Tucker, 1951), it was proved that the optimum found for the global RSM model was a global optimum. In this study, four initial conditions were tested for convergence of the global approach. The initial designs tested were $[x_1, x_2, x_3, x_4, x_5, x_6, x_7]$ = [0,0,0,0,0,0,0], [1,1,1,1,1,1,1], [-1,-1,-1,-1, -1,-1,-1], and [-0.8,-0.8,-0.8, 0.8,0.8,-0.8,0.8]. Using the MATLAB program as shown in Appendix A, all of these initial designs led to the single optimal design. The proof of global convergence for quadratic global RSM model is given in Appendix B.

On the other hand, the local approach did not exhibit such a global convergence. It yielded non-unique termination points, but with essentially equivalent objective values. Furthermore, it converged after only two iterations and required less effort that running the 62 simulations of Table 5.3 to find the Global RSM model. With ASPEN PLUS,

Table 5.13 Comparison of optimization results from alternative approaches: all yields calculated using ASPEN PLUS

Conditions	Decision Variables							Yield (y)
	x_1	x_2	x_3	x_4	x_5	x_6	x_7	
Nominal design	0	0	0	0	0	0	0	486,591.22
Best of experimental results	0	-1	-1	0	0	-1	0	513,783.90
Final ASPEN design: case# 1	0	0	-1	0.8	0	-1	0	522,297.59
Final ASPEN design: case# 2	-0.8	-0.8	-1	0.8	0.8	-1	0.8	522,576.15
Global (RSM model) optimal design	-1	-1	-1	1	1	-1	1	523,798.53

Note : Case# 1-Initial condition = [0,0,0,0,0,0,0].
Case# 2-Initial condition = [-0.8,-0.8,-0.8,0.8,0.8,-0.8,0.8].

Table 5.14 Comparison of yields from the CHEMCAD model, the global RSM model and the ASPEN PLUS model

Conditions	Yields (US$/day)		
	CHEMCAD III	RSM model	ASPEN PLUS
Nominal design	482,061.57	482,401.00	486,591.22
Best of experimental results	504,698.76	504,176.23	513,783.90
Global (RSM model) optimal design	515,610.71	515,070.05	523,798.53

computation times required for one simulation run or one optimization run were about 3 and 27 seconds, respectively. Thus, the total simulation time required for the global approach (62 simulation runs) was about 186 seconds or approximately 7 times more computing time than the local approach. Since the Box-Behnken modeling is not automated, the time to set up the modeling simulations and calculate the quadratic parameters was an additional burden in the global approach implementation.

Chapter 6

Conclusions and Recommendations

6.1 Process Conclusions

The results of process optimization via global and local approaches presented in Chapter 5 indicated that maximum total sales for the offshore natural gas process could be achieved by readjusting three design variables, which had significant effects on objective function. In the natural gas processing problem, the objective function effectively depended on only three design variables: the compression ratio of the Production Compressor, the heat duty of the Gas/Gas Exchanger and the compression ratio of the Expander. The maximum total sales was obtained by using the minimum compression ratios of the Production Compressor and the Expander, and maximum heat duty for the Gas/Gas Exchanger. This combination of the three variables tended to increase the production of raw condensate and decrease production of sales gas compared to the nominal design, and this could be taken as a reasonable operating principle to ensure profitability.

Figure 6.1 shows the flow diagram of the process at optimal design conditions. It can be seen that the production rate of condensate increased tremendously in the Dew Point Control Unit (DPCU), while the production of condensate from other units remained approximately the same. The production rate of condensate from the DPCU at optimal conditions was about 160% more than the production rate at nominal design conditions.

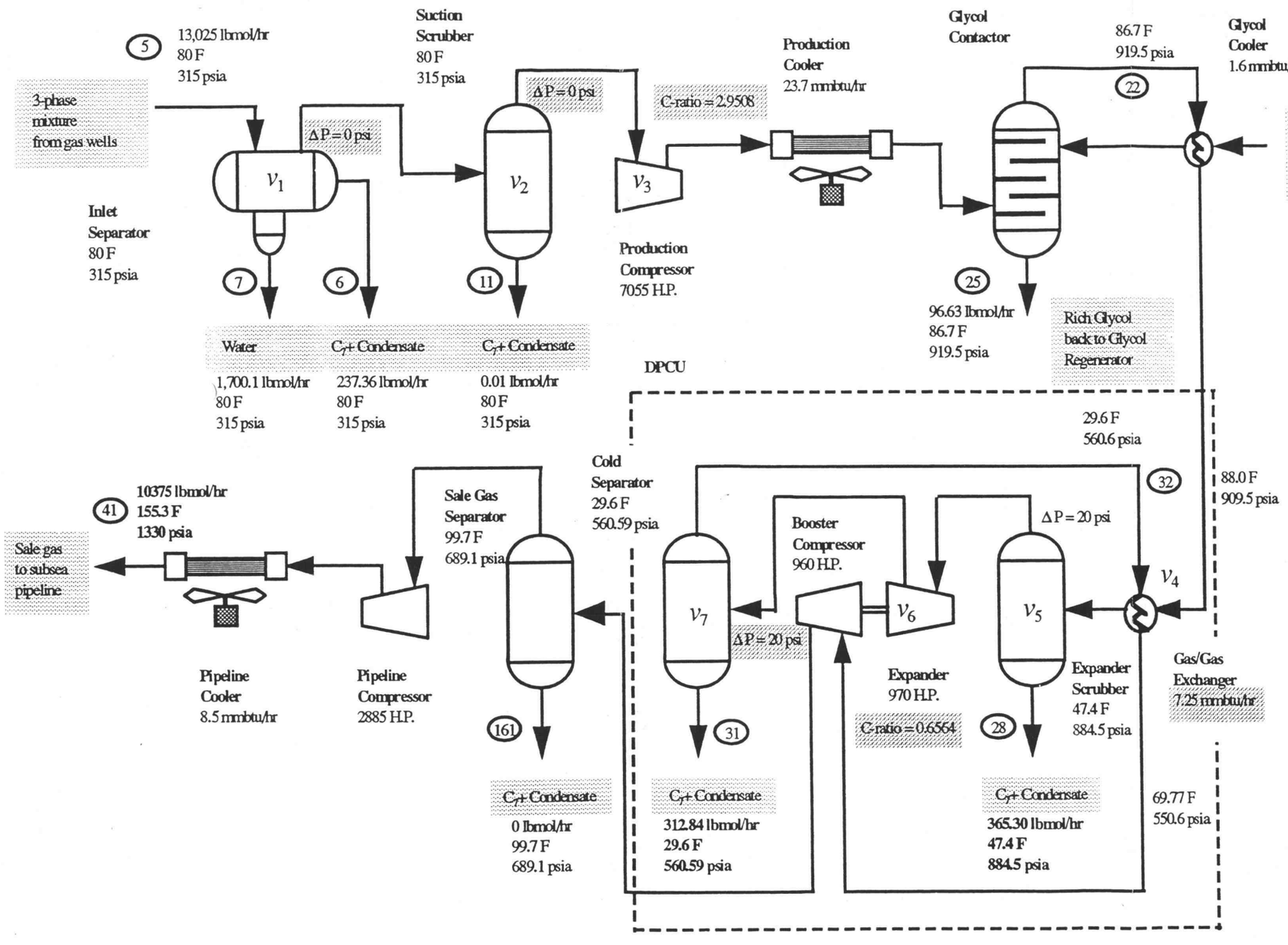

Figure 6.1 Flow diagram of the natural gas process - optimal design (ASPEN PLUS)

The condensate production at the Expander Scrubber and the Cold Separator increased by 180% and 140%, respectively. On the other hand, the production rate and heating value of sale gas decreased by just 4% and 1%. For the objective values, gas sale decreased by 6%, condensate sale increased by 60%, and total sales increased by about 8%. This is an obvious indication that the condensate production should be favored over the gas production in this study.

To increase the condensate production, the dew point of sale gas was lowered so that more heavy hydrocarbons condensed in the process, especially at the DPCU. The compression ratio of the Production Compressor and the heat duty of the Gas/Gas Exchanger had major effects on the gas condensation in the Expander Scrubber, while the compression ratio of the Expander significantly affected the gas condensation in the Cold Separator. From an operational standpoint, all units positioned before the DPCU should be operated at as low pressure as possible, all available heat exchanger area in the Gas/Gas Exchanger should be fully utilized, and each unit inside the DPCU should have as a high pressure drop as possible, in order to maximize production of raw condensate and total sales. The gas flow from the DPCU had to be pressurized to the pipeline pressure level at the Pipeline Compressor, thus lower pressures in the DPCU would have an undesirable effect of increasing the required power used in the Pipeline Compressor.

Note that operating pressure is related to flow rate and size of an equipment. Since the sizes of process equipment were considered fixed, the flow rate in each unit was directly affected by the operating pressure. This effect could not be observed from the

simulation results because the process modules used were based on steady-state equilibrium calculations.

In summary, there were three design variables that had significant effects on the objective value of the offshore natural gas process. The combination of these three variables tended to maximize the production of raw condensate by lowering the dew point of sale gas. Although some effects of flow rate on process parameters were not incorporated in commercial process simulators, the results of this optimization study should provide useful guidance for on-line experiments to improve the real process.

6.2 Simulation Recommendations

The optimization results suggested that the global approach to optimization required more engineering time to set up, but once the quadratic model was found the optimal solution was easy to compute. In the natural gas processing problem, the successive local approximation approach was more attractive because it gave comparable results to those from the global approach while requiring considerably less effort to implement.

The global approach was more robust because the global model optimum was easy to compute and the choice of initial design did not affect the convergence. The additional insight of the process behavior gained from running case studies might be useful for an inexperienced engineer, but such studies would be more useful once an optimal design has been found. When more design variables are included in the optimization, substantially more process simulations would be needed to identify the RSM model.

Although the local approach did not converge for all initial designs, when it did it required much fewer flowsheet evaluations. Experienced engineers should be able to choose good initial designs to avoid any convergence problems.

For this problem, the SQP capability of ASPEN PLUS was sufficient for identifying the three major design variables and the best way to operate the process. This process had a relatively flat objective function with substantial differences in the effects of design variables, so that the success of the local approach was as expected. It would be interesting to study optimization of a process where local maxima arose were significantly better than surrounding regions but distinct from each other.

Comparisons of simulation results from CHEMCAD III and ASPEN PLUS presented in Chapter 5 showed that the use of different process simulators had little effect on the value of the optimal objective or on the optimal values of design variables. The differences in their simulation results were caused by small differences in the thermodynamic calculation package, unit operation modules, physical property data and calculation methods.

For process optimization studies using simulators, it is best to choose only variables which have significant effects on the objective function as design variables. At the beginning of a project, however, this is one of the questions to be answered by optimization study. Such variable screening task can be done by performing sensitivity analyses via case studies on each variable starting at a nominal design. A better approach, however, might be to first utilize the SQP capability to find at least a locally optimal design to serve as the nominal design. Engineering judgment should always be applied to

the selection of design variables, but newly incorporated optimization capabilities of process simulators offer additional engineering tools to help produce good process designs.

6.3 Future Research Areas

The following are research areas recommended for further studies.

1) An improved objective function that reflect more accurately the operating costs of running the DPCU unit at lower pressure and using a larger pipeline compressor should be used for further studies of the natural gas process.

2) A process with material as well as energy recycle streams, such as a reactor/separation scheme to recycle unreacted feed back to the reactor, is recommended for studies of ASPEN PLUS's SQP capabilities.

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APPENDICES

Appendix A

MATLAB Computer Program and Results

The following is a MATLAB computer program written to solve the optimization problem derived from the global approach. This program consists of two files, *Optmax.m* and *Yields2.m*. *Optmax.m* is a main M-file for solving the problem, while *Yields2.m* is an M-file defining the objective function and its gradient. The built-in MATLAB function used in Optmax.m was "*constr*( )", which was designed to find the minimum of a constrained multivariable function using an SQP method (MATLAB Optimization Toolbox user's guide, 1990). An estimate of the Hessian of the Lagrangian is updated at each iteration using the Broyden-Fletcher-Golfarb-Shanno (BFGS) formula. A line search is performed using a merit function similar to that proposed by Han (1977) and Powell (1978).

This optimization was run starting at four different initial design points and each run converged to the same solution. Those initial designs were:

Case #1 : $[x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [0,0,0,0,0,0,0]$, the nominal design

Case #2 $[x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [1,1,1,1,1,1,1]$

Case #3 $[x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [-1,-1,-1,-1,-1,-1,-1]$

Case #4 $[x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [0,0-1,1,0,-1,0]$

Optmax.m

```
echo on
%-------------------------------------------------------------------------
%  This program is to compute the maximum value of the objective
%  function obtained from the response surface analysis.
%-------------------------------------------------------------------------
echo off
disp(' ')
disp('Enter initial design variable values:')
disp(' ')
disp(' ')
X1 = input('Initial X1:');
X2 = input('Initial X2:');
X3 = input('Initial X3:');
X4 = input('Initial X4:');
X5 = input('Initial X5:');
X6 = input('Initial X6:');
X7 = input('Initial X7:');
X = [X1 X2 X3 X4 X5 X6 X7];
options = [];
VLB = [-1 -1 -1 -1 -1 -1 -1];
VUB = [ 1  1  1  1  1  1  1];
X_MAX = constr('yield2',X,options,VLB,VUB);
[Y,g] = yield2(X_MAX);
disp(' ')
disp('Hit any key to see optimal design variables and corresponding yield:')
pause
disp(' ')
disp(' ')
disp(sprintf('X1 = %5.3f',X_MAX(1)))
disp(sprintf('X2 = %5.3f',X_MAX(2)))
disp(sprintf('X3 = %5.3f',X_MAX(3)))
disp(sprintf('X4 = %5.3f',X_MAX(4)))
disp(sprintf('X5 = %5.3f',X_MAX(5)))
disp(sprintf('X6 = %5.3f',X_MAX(6)))
disp(sprintf('X7 = %5.3f',X_MAX(7)))
disp(' ')
disp(sprintf('The maximum yield = %8.2f', -Y))
```

Yield2.m

```
function [Y,g] = yield2(X)

Y =     -(482401.00 + 398.26*X(1) + 562.13*X(2) - 9622.93*X(3) + 7738.03*X(4)...
        + 200.22*X(5) - 10219.00*X(6) + 357.38*X(7) + 137.30*(X(1)^2)...
        - 29.68*(X(2)^2) + 1102.24*(X(3)^2) - 812.91*(X(4)^2) + 93.18*(X(5)^2)...
        + 805.94*(X(6)^2) - 96.86*(X(7)^2) - 68.91*X(1)*X(2) + 198.10*X(1)*X(3)...
        + 60.96*X(1)*X(4) - 17.02*X(1)*X(5) + 536.21*X(1)*X(6) - 8.00*X(1)*X(7)...
        + 238.53*X(2)*X(3) + 54.39*X(2)*X(4) - 15.26*X(2)*X(5)...
        + 537.28*X(2)*X(6) - 20.03*X(2)*X(7) - 1903.68*X(3)*X(4)...
        + 17.27*X(3)*X(5) - 158.88*X(3)*X(6) - 98.77*X(3)*X(7)...
        + 32.64*X(4)*X(5) - 1340.11*X(4)*X(6) - 62.62*X(4)*X(7)...
        + 162.50*X(5)*X(6) - 2.31*X(5)*X(7) + 65.12*X(6)*X(7));

g = [];
```

Results

Case #1

```
%-------------------------------------------------------------------------
% This program is to compute the maximum point of the
% empirical model obtained from response surface analysis.
%-------------------------------------------------------------------------
echo off

Enter initial guesses for optimum condition:
Initial X1:0
Initial X2:0
Initial X3:0
Initial X4:0
Initial X5:0
Initial X6:0
Initial X7:0

Hit any key to see optimum condition and yield:

X1 = -1.000
X2 = -1.000
X3 = -1.000
X4 =  1.000
X5 =  1.000
X6 = -1.000
X7 =  1.000

The maximum yield = 515,070.05
```

Case #2

```
%-------------------------------------------------------------------------
% This program is to compute the maximum point of the
% empirical model obtained from response surface analysis.
%-------------------------------------------------------------------------
echo off

Enter initial guesses for optimum condition:
Initial X1:1
Initial X2:1
Initial X3:1
Initial X4:1
Initial X5:1
Initial X6:1
Initial X7:1

Warning: Matrix is close to singular or badly scaled.
         Results may be inaccurate. RCOND = 4.102977e-030

Hit any key to see optimum condition and yield:

X1 = -1.000
X2 = -1.000
X3 = -1.000
X4 =  1.000
X5 =  1.000
X6 = -1.000
X7 =  1.000

The maximum yield = 515,070.05
```

Case #3

```
%-------------------------------------------------------------------------
% This program is to compute the maximum point of the
% empirical model obtained from response surface analysis.
%-------------------------------------------------------------------------
echo off
Enter initial guesses for optimum condition:

Initial X1:-1
Initial X2:-1
Initial X3:-1
Initial X4:-1
Initial X5:-1
Initial X6:-1
Initial X7:-1

Hit any key to see optimum condition and yield:

X1 = -1.000
X2 = -1.000
X3 = -1.000
X4 =  1.000
X5 =  1.000
X6 = -1.000
X7 =  1.000

The maximum yield = 515,070.05
```

Case #4

```
%-------------------------------------------------------------------------
% This program is to compute the maximum point of the
% empirical model obtained from response surface analysis.
%-------------------------------------------------------------------------
echo off
Enter initial guesses for optimum condition:

Initial X1:0
Initial X2:0
Initial X3:-1
Initial X4:1
Initial X5:0
Initial X6:-1
Initial X7:0

Hit any key to see optimum condition and yield:

X1 = -1.000
X2 = -1.000
X3 = -1.000
X4 =  1.000
X5 =  1.000
X6 = -1.000
X7 =  1.000

The maximum yield = 515,070.05
```

Appendix B

Proof of Global Convergence for Quadratic Global RSM Model

The optimization problem statement for the quadratic global RSM model, Equation 3.2, can be stated as:

Minimize $\theta(\underline{x})$ (B.1)

Subject to $\underline{g}(\underline{x}) \leq 0$

where,

$$\theta(\underline{x}) = -\left(\beta_0 + \sum_{i=1}^{7} \beta_i x_i + \sum_{i=1}^{7} \beta_{ii} x_i^2 + \sum_{\substack{i=1 \\ i<j}}^{7} \sum_{j=1}^{7} \beta_{ij} x_i x_j \right)$$

$$g_{i,1} = x_i - 1 \leq 0$$

$$g_{i,2} = -x_i - 1 \leq 0$$

Referring to Mangasarian (1979), the Kuhn-Tucker (KT) necessary optimality criteria must be satisfied in order to assure a global solution of Equation B.1. The Kuhn-Tucker (KT) necessary optimality criteria for Equation B.1 are;

$$\nabla\theta(\bar{x}) + \bar{\underline{u}}\nabla\underline{g}(\bar{x}) = 0 \quad \text{(B.2-a)}$$

$$g_i(\bar{x}) \leq 0, \quad \text{all } i \quad \text{(B.2-b)}$$

$$\bar{u}\underline{g}(\bar{x}) = 0 \qquad \text{(B.2-c)}$$

$$\bar{u}_i \geq 0, \text{ all } i \qquad \text{(B.2-d)}$$

At the optimal point (as an equality), $\bar{x}$ = [-1, -1, -1, 1, 1, -1, 1], obtained from the RSM model, Equation B.2-b is satisfied, and so is Equation B.2-c. Since $\theta(x)$, $\underline{g}(x)$ and $\bar{x}$ were known, $\bar{u}$ was obtained by solving Equation B.2-a using MATLAB. Equation B.2-d was satisfied by the solution found as $\bar{u}$ = [506, 66, 14090, 9211, 269, 13858, 160]. This indicated that the Kuhn-Tucker (KT) necessary optimality criteria were satisfied.

For the sufficient optimality condition, the Hessian of the objective function must be negative definite everywhere (for maximization problem) and the constants must be linear. The Hessian can then be symbolically written as;

$$\underline{H}(\underline{x}) \equiv \nabla^2 f(\underline{x}) = \begin{bmatrix} \frac{\partial^2 f(\underline{x})}{\partial x_1^2} & \frac{\partial^2 f(\underline{x})}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(\underline{x})}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(\underline{x})}{\partial x_2 \partial x_1} & & & \vdots \\ \vdots & & & \vdots \\ \frac{\partial^2 f(\underline{x})}{\partial x_n \partial x_1} & \cdots & \cdots & \frac{\partial^2 f(\underline{x})}{\partial x_n^2} \end{bmatrix} \qquad \text{(B.3)}$$

The Hessian is negative definite when all of its eigenvalues are negative. Calculation of the constant eigenvalues was done using MATLAB. The results showed that all eigenvalues of the Hessian matrix were negative, [-179.5,-191.4,-69.7,-440.7,-1795.8,

-815.8,-4294.8]. Thus, the sufficient optimality condition was satisfied and the local maximum found using MATLAB *constr*( ) procedure must be the global solution of Equation 3.1.

Appendix C

Statistical Parameters for RSM Results

The following are formulae used for statistical analysis of the Box-Behnken designs shown in Table 3.3. These formulae were derived by Box and Behnken (1960). Values of constants and notation of terms used in these formulae are given in Chapter 3.

Variance and Covariance

$$V(\beta_0) = \frac{1}{n_0}\sigma^2 \tag{C.1}$$

$$V(\beta_i) = A\sigma^2 \tag{C.2}$$

$$V(\beta ii) = \left[B + 1/s^2 n_0\right]\sigma^2 \tag{C.3}$$

$$V(\beta_{ij}) = D\sigma^2 \tag{C.4}$$

$$\mathrm{Cov}(\beta_0 \beta_{ii}) = -\frac{1}{s^2 n_0}\sigma^2 \tag{C.5}$$

$$\mathrm{Cov}(\beta_{ii} \beta_{jj}) = \left[C + \frac{1}{s^2 n_0}\right]\sigma^2 \tag{C.6}$$

Note that $V(i)$ and $\mathrm{Cov}(i)$ are variance and covariance of coefficient i, respectively.

Analysis of Variance

Correction due to the mean: $\{0y\}^2/N$ (C.7)

Sum of squares due to linear terms: $A\sum_{i=1}^{k}\{iy\}^2$ (C.8)

Sum of squares due to second degree terms: (C.9)

a) Due to interaction terms $D\sum_{i<j}^{n_1}\{ijy\}^2$

b) Due to quadratic terms $\beta_0\{0y\}+\sum_{i=1}^{k}\beta_{ii}\{iiy\}-\{0y\}^2/N$

Total sum of squares after correction for the mean: (C.10)

$$\sum_{u=1}^{N}y_u^2-\{0y\}^2/N$$

Appendix D

Development of SQP Algorithm

In this appendix, a brief development of the general Successive Quadratic Programming (SQP) algorithm is given. For further details, nonlinear programming textbooks are recommended. Note that SQP is also known as *Sequential Quadratic Programming*.

The Lagrange-Newton Equations (equality constraints)

Before addressing the general NLP with equality and inequality constraints, first consider the minimization problem with only equality constraints.

$$\begin{aligned} &\min \quad \theta(\underline{x}) \\ &\text{subject to} \quad \underline{h}(\underline{x}) = 0 \end{aligned} \tag{D.1}$$

The Lagrangian for this problem is an augmented objective function defined as:

$$L(\underline{x},\underline{u}) = \theta(\underline{x}) + \sum_{i=1}^{n} u_i h_i(\underline{x}) \tag{D.2}$$

where L and $\underline{u}$ are the Lagrangian function and the Lagrange multiplier vector associated with the equality constraints respectively.

The stationary condition for the Lagrangian of this problem with respect to both $\underline{x}$ and $\underline{u}$ is then $\underline{\nabla L}(\underline{x}_*, \underline{u}_*) = \underline{0}^T$. Newton's method may be chosen to update $\underline{x}$ and $\underline{u}$ to solve these equations. This is done by using the Taylor expansion to first order

$$\nabla L_{k+1}^T = \left[\underline{\nabla} L(\underline{x}_k + \delta \underline{x}_k, \underline{u}_k + \delta \underline{u}_k\right]^T = \underline{\nabla} L_k^T + \underline{\underline{\nabla}}^2 L_k (\delta \underline{x}_k, \delta \underline{u}_k)^T \qquad \text{(D.3)}$$

and setting the left-hand side $\nabla L_{k+1}^T = 0$. Then Equation (D.3) gives

$$\nabla^2 L_k \begin{pmatrix} \delta \underline{x}_k \\ \delta \underline{u}_k \end{pmatrix} = -\nabla L_k^T \qquad \text{(D.4)}$$

It is computed easily that

$$\nabla^2 L_k = \begin{pmatrix} \nabla_x^2 L & \nabla_{xu}^2 L \\ \nabla_{ux}^2 L & \nabla_u^2 L \end{pmatrix}_k = \begin{pmatrix} \nabla^2 \theta + \underline{u}^T \nabla^2 \underline{h} & \nabla \underline{h}^T \\ \nabla \underline{h} & 0 \end{pmatrix}_k \qquad \text{(D.5)}$$

$$\nabla L_k = \left(\nabla \theta^T + \nabla \underline{h}^T u, \underline{h}\right)_k^T \qquad \text{(transposed element)} \qquad \text{(D.6)}$$

Define further for convenience the shorthand

$$\underline{\underline{W}} = \nabla^2\theta + \underline{u}^T\nabla^2\underline{h}, \qquad \underline{\underline{A}} = \nabla\underline{h} \tag{D.7}$$

Then Equation (D.4) can be rewritten as

$$\begin{pmatrix} \underline{\underline{W}}_k & \underline{A}_k^T \\ \underline{A}_k & \underline{0} \end{pmatrix}\begin{pmatrix} \delta\underline{x}_k \\ \delta\underline{u}_k \end{pmatrix} = \begin{pmatrix} -\nabla\theta_k^T - \underline{\underline{A}}_k^T\underline{u}_k \\ -\underline{h}_k \end{pmatrix} \tag{D.8}$$

Setting $\delta\underline{x}_k = \underline{s}_k$ (search step vector) and $\delta\underline{u}_k = \underline{u}_{k+1} - \underline{u}_k$, Equation (D.8) can be simplified to

$$\begin{pmatrix} \underline{\underline{W}}_k & \underline{A}_k^T \\ \underline{A}_k & \underline{0} \end{pmatrix}\begin{pmatrix} \underline{s}_k \\ \underline{u}_{k+1} \end{pmatrix} = \begin{pmatrix} -\nabla\theta_k^T \\ -\underline{h}_k \end{pmatrix} \tag{D.9}$$

Solving Equation (D.9) iteratively, we obtain the iterants $\underline{x}_{k+1} = \underline{x}_k + \underline{s}_k$ and $\underline{u}_{k+1}$, which eventually should approach $\underline{x}_*$ and $\underline{u}_*$. Thus, any method solving Equation (D.9) can be referred to as a *Lagrange-Newton* method for solving the constrained problem (D.1). The solution can be shown to be unique if $\underline{\underline{A}}_*$ has full rank (regularity assumption) and $\underline{\underline{W}}_*$ is positive-definite on the tangent subspace (Papalambros and Wilde, 1988).

Equation (D.9) may be written explicitly as

$$\underline{\underline{W}}_k\underline{s}_k + \underline{\underline{A}}_k^T\underline{u}_{k+1} + \nabla\theta_k^T = 0 \tag{D.10}$$

$$\underline{\underline{A}}_k\underline{s}_k + \underline{h}_k = 0$$

and Equation (D.10) may be viewed as the Karush-Kuhn-Tucker (KKT) conditions, which are the necessary optimality conditions for an optimization problem, for the quadratic model

$$\begin{aligned} \min \quad & q(\underline{s}_k) = \theta_k + \nabla_x L_k \underline{s}_k + \frac{1}{2} \underline{s}_k^T \underline{\underline{W}}_k \underline{s}_k \\ \text{subject to} \quad & \underline{\underline{A}}_k \underline{s}_k + \underline{h}_k = 0 \end{aligned} \tag{D.11}$$

where $\nabla_x L_k = \nabla\theta_k + \underline{u}_k^T \nabla \underline{h}_k$ and the multipliers of problem (D.11) are $\delta \underline{u}_k$. In fact, the Lagrangian stationary condition of (D.11) is

$$\nabla_x L_k + \underline{s}_k^T \underline{\underline{W}}_k + (\delta \underline{u}_k)^T \underline{\underline{A}}_k = \underline{0}^T$$

or, transposing,

$$\nabla\theta_k^T + \underline{\underline{A}}_k^T \underline{u}_k + \underline{\underline{W}}_k \underline{s}_k + \underline{\underline{A}}_k^T (\underline{u}_{k+1} - \underline{u}_k) = \underline{0} \tag{D.12}$$

which is easily reduced to the first line of equation (D.10). Thus, the solution of the quadratic programming subproblem, equation (D.11), gives $\underline{s}_k$ and $\underline{u}_{k+1}$ which also satisfy Equation (D.10), and the two formulations are equivalent. If the second formulation is selected for solving the Lagrange-Newton equation, the values of $\underline{x}_*$ and $\underline{u}_*$ will be

obtained from solving a sequence of quadratic programming (QP) subproblems, hence the relevant algorithms are known as *successive quadratic programming* (SQP) methods. The QP subproblem may not be exactly as in (D.11). For example, the subproblem

$$\begin{aligned} \min \quad & q(\underline{s}_k) = \theta_k + \nabla\theta_k \underline{s}_k + \frac{1}{2}\underline{s}_k^T \underline{\underline{W}}_k \underline{s}_k \\ \text{subject to} \quad & \underline{\underline{A}}_k \underline{s}_k + \underline{h}_k = 0 \end{aligned} \tag{D.13}$$

also gives a solution $\underline{s}_k$ and multiplier $\underline{u}_{k+1}$ directly, rather than $\delta\underline{u}_k$ as (D.11) does.

A simple SQP algorithm has the following general structure.

SQP algorithm (without line search)

1. Select initial point $\underline{x}_0$, $\underline{u}_0$; let $k = 0$.
2. For $k = k+1$, solve the QP subproblem and determine $\underline{s}_k$ and $\underline{u}_{k+1}$.
3. Set $\underline{x}_{k+1} = \underline{x}_k + \underline{s}_k$.
4. If termination criteria are not satisfied, return to 2.

Enhancements of the Basic Algorithm

The QP subproblem (D.11) minimizes the quadratic approximation to the Lagrangian subject to the linearized constraints. A solution exists if $\underline{\underline{W}}_k$ is positive-definite, a condition implicit in equation (D.9) for stability of Newton's method. Local

convergence of the algorithm can be proven to be quadratic if $\underline{\underline{W}}_k$ behaves properly. The difficulty, however, is with global convergence. For points far from $\underline{x}_*$, the QP subproblem may have an unbounded or infeasible solution. A stabilization procedure must be implemented. One possibility is to view $\underline{s}_k$ as only a search direction and define the iteration as $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{s}_k$ where the step size α_k results from minimizing an appropriate function along the search direction. This function, called a *merit function*, should measure how good $\underline{s}_k$ and $\underline{u}_k$ are (including feasibility), and should be locally minimized at the solution. This suggests some form of penalty function that properly weighs an objective function decrease and avoidance of constraint violations. Only penalizing constraint violations could lead to stationary points that are not minimum points. For example, the merit function

$$\phi(\underline{x},\underline{u}) = \left\|\nabla_x L(\underline{x},\underline{u})\right\|^2 + \left\|\underline{h}(\underline{x})\right\|^2 \qquad \text{(D.14)}$$

representing the KKT conditions' violation would not be very satisfactory. The solution of a proper function is a currently active area of research (Papalambros and Wilde, 1988).

Another point of practical interest is the evaluation of the matrix $\underline{\underline{W}}_k$ in the QP subproblem. The obvious enhancement is to avoid estimating second derivatives from function evaluations by employing an updating formula that approximates $\underline{\underline{W}}_k$ as in the quasi-Newton method. One possibility is to use the Davidon-Fletcher-Powell (DFP) formula with $\delta \underline{g}_k$ defined as:

$$\delta \underline{g}_k = \nabla L(x_{k+1}, u_{k+1})^T - \nabla L(x_k, u_{k+1})^T \tag{D.15}$$

Another possibility is to use the Broyden-Fletcher-Goldfarb-Shanno (BFGS) formula and keep the approximating matrix positive-definite by using the linear combination

$$\delta \underline{g}_k = \beta_k \underline{y}_k + (1-\beta_k)\underline{\underline{H}}_k \delta \underline{x}_k, \quad 0 \le \beta \le 1 \tag{D.16}$$

in the BFGS approximation to the Hessian of the Lagrangian, where

$$\underline{y}_k = \nabla L(\underline{x}_{k+1}, \underline{u}_{k+1})^T - \nabla L(\underline{x}_k, \underline{u}_{k+1})^T \tag{D.17}$$

$$\beta_k = \begin{cases} 1 & \text{if } \delta \underline{x}_k^T \underline{y}_k \ge (0.2)\delta \underline{x}_k^T \underline{\underline{H}}_k \delta \underline{x}_k \\ \dfrac{(0.8)\delta \underline{x}_k^T \underline{\underline{H}}_k \delta \underline{x}_k}{\delta \underline{x}_k^T \underline{\underline{H}}_k \delta \underline{x}_k - \delta \underline{x}_k^T \underline{y}_k} & \text{if } \delta \underline{x}_k^T \underline{y}_k < (0.2)\delta \underline{x}_k^T \underline{\underline{H}}_k \delta \underline{x}_k \end{cases}$$

$\underline{\underline{H}}$ = Hessian matrix of the objective function

The values 0.2 and 0.8 were chosen based on numerical experiments. The choice of β_k is made to assure that $\delta \underline{g}_k$ remains as close to $\underline{y}_k$ as possible, while $\delta \underline{x}_k^T \underline{y}_k \ge (0.2)\delta \underline{x}_k^T \underline{\underline{H}}_k \delta \underline{x}$ is always satisfied. That way, $\delta \underline{x}^T \delta \underline{g}_k > 0$ is preserved and $\underline{\underline{H}}_{k+1}$ will always be positive definite if $\underline{\underline{H}}_k$ is as well.

In the construction above, $\delta \underline{x}_k$ is the search direction $\underline{s}_k$ if no line search is performed. However, when a merit function is used for line search, $\delta \underline{x}_k = \alpha_k \underline{s}_k$ and the updating of $\underline{\underline{H}}_k$ is done after the line search is completed. The new $\underline{\underline{H}}_{k+1}$ approximate $\underline{\underline{W}}_{k+1}$ in the next QP subproblem (D.11) or (D.13).

An alternative to solving the QP subproblem is to solve a linear least squares subproblem based on a Cholesky $\mathbf{LDL}^T$ factorization of the approximating Hessian (Schittkowski, 1981).

Inclusion of Inequality Constraints

The previous presentation of the SQP algorithm included only equality constraints. For the general NLP problem

$$\begin{aligned} \min \quad & \theta(\underline{x}) \\ \text{subject to} \quad & \underline{h}(\underline{x}) = 0 \\ & \underline{g}(\underline{x}) \le 0 \end{aligned} \tag{D.18}$$

the inequality constraints may be treated using two different methods. First, an active set strategy may be employed on the original problem (D.18) so that the QP subproblem of inner iteration will be always only equality constrained. This is sometimes called a *pre-assigned active set strategy* in SQP. The merit function must then include all constraints, active and inactive, to guard against failure when the wrong active set is used to determine $\underline{s}$. The second treatment is to pose the QP subproblem with the linearized inequalities

included, that is, $\underline{\underline{A}}_k \underline{s}_k + \underline{g}_k \leq \underline{0}$, and use an active set strategy on the QP subproblem. The resulting active set for the original problem may be employed as a prediction of the active set for the original problem, but it is not yet clear if this is in fact an advantage over the first method.

In summary, current SQP algorithms have the following steps.

SQP Algorithm (with line search)

1. Initialize
2. Solve the QP subproblem to determine a search direction $\underline{s}_k$
3. Minimize a merit function along $\underline{s}_k$ to determine a step length α_k
4. Set $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{s}_k$
5. Check for termination criteria. Go to 2 if not satisfied.

Scaling

Scaling is a term often used loosely to describe numerical difficulties that may be associated with large differences in the values of computed quantities, usually of many orders of magnitude, but also associated with computing values that may be too small to distinguish from each other or from a practical zero value, that is, some quantity ε in the finite arithmetic of digital computers. In optimization algorithms, scaling can be critical when actual design models are used because in these cases the design quantities are expressed in units natural for the problem at hand. In general, a model should be scaled

with respect to its variables, so that *all variables have similar magnitudes in value, and preferably of order one, in the feasible domain.*

Scaling can be viewed as a linear transformation of the form

$$\underline{z} = \underline{\underline{A}}\underline{x} + \underline{b} \tag{D.19}$$

where $\underline{\underline{A}}$ is a nonsingular matrix and $\underline{b}$ is a nonzero vector. Thus, the coordinate system $\underline{x}$ is replaced by the coordinate system $\underline{z}$. Since $\underline{\underline{A}}$ is assumed nonsingular, it is invertible and the transformation is one to one. It is easy to prove that under a linear transformation we get

$$\nabla_x \theta = (\nabla_z \theta)\underline{\underline{A}}, \quad \nabla_x^2 = \underline{\underline{A}}^T (\nabla_z^2 \theta)\underline{\underline{A}} \tag{D.20}$$

An optimization algorithm is called *invariant* under the linear transformation, if $\underline{z}_k = \underline{\underline{A}}\underline{x}_{k+1} + \underline{b}$. The invariance property is theoretically significant because invariant algorithms tend to be insensitive to ill-conditioning. Note that any algorithm that takes the identity matrix $\underline{\underline{I}}$ as an approximation to the Hessian will *not* be invariant. Thus, the gradient method, the modified Newton with stabilization, and quasi-Newton methods with $\underline{\underline{H}}_0 = \underline{\underline{I}}$ are not invariant, but theoretically Newton's method with a line search will be invariant. In practice, no algorithm is truly invariant and the property is only marginally useful (Peressini, Sullivan, and Uhl, 1987).